TOGETHER FOR SUSTAINABILITY

The Product Carbon Footprint Guideline for the Chemical Industry

Specification for Product Carbon Footprint and Corporate Scope 3.1 Emission Accounting and Reporting

Version 3.0 - December 2024

The PCF Guideline from Together for Sustainability

Across the chemical industry, there is an urgent need to decarbonize – especially in the value chain, beyond a corporation's own operations (Scope 3). Currently, a major share of the industry's greenhouse gas (GHG) emissions arises from the upstream value chain. Increasing data transparency and accuracy on the product-level is a key element to drive emission reductions along the value chain and is a strategic cornerstone of many corporate climate mitigation strategies.

The TfS PCF Guideline is unique in that it draws on the wealth of expertise and knowledge within the TfS member network to develop norms for the chemical industry, while remaining fully compliant with existing methods including ISO and the Greenhouse Gas Protocol. The PCF Guideline will create benefits for TfS members, their suppliers, as well as other industries initiatives as a drop-in solution for the chemical sector.

By applying the PCF Guideline, TfS members and their value chain partners can holistically approach the integration of PCFs of chemical products within their corporate GHG inventories, with a focus on Scope 3 Category 1 (Purchased Goods and Services) emissions. The comprehensive guideline instructs companies on how to calculate and share the PCFs of their own chemical products. It also provides guidance on how to calculate corporate Scope 3.1 inventories on the basis of supplier-specific data, supporting transparency and decarbonize the entire value chain.

About this version

Originally published in 2022, this 2024 update marks the third version of the TfS PCF Guideline. This version adds new information to Chapter 5 on the PCF calculation of mass-balanced products. It also includes a new section in Chapter 4 with guidance on Scope 3 baseline restatement for companies with Scope 3 climate targets. Additionally, there have been changes to several subchapters such as Carbon Capture and Utilization identification and calculation of waste from multi output processes with a new decision tree, calculation of mass balance products or a new and harmonized approach of the assessment of data quality and primary data shares.

The TfS PCF Guideline will continue to evolve as needed to maintain alignment with key carbon accounting methodologies and GHG reporting requirements. TfS occasionally releases additional information and thought leadership to inform GHG accounting and reporting, such as the TfS White Paper: Improving and Harmonising Scope 3 Reporting. Please visit the **TfS website** to view recent Publications.

This section of the Guideline document provides a comprehensive overview of the changes made since the previous edition, including the rationale behind them and a concise summary of their technical descriptions. It is designed to assist readers familiar with earlier versions in tracking these updates and understanding the driving factors for the changes.

For readers new to this document, this section also serves as a valuable reference for understanding the evolution of the different versions of the Guideline over time. While the document has achieved significant alignment with other guidelines, some of the newer and more complex methodological elements will continue to evolve to meet emerging industry and cross-industry needs. This iterative approach ensures that the TfS Guideline remain aligned with current requirements for Product Carbon Footprint and Scope 3 accounting calculations of generic standards.

In addition to the detailed changes outlined in Table E.1, minor editorial corrections have been made, though these are not specifically listed here.

Table E.1: Summary of key changes of this new version 3 (2024) vs. The Product Carbon Footprint Guideline for the Chemical Industry version 2.1 (2022) and 2.2 (2023)

Topic:	"Where to find" in v2.1 and 2.2 document:	"Where to find" in v3 document:	Description of the changes:	Summary of the changes and technical justification driving the change(s):
1. Carbon Capture and Storage or Utilization	Chapter 5.2.10.4 (page 74)	Chapter 5.2.10.4 (page 85)	This chapter has been re-written with consideration of more consistent approaches for handling of credits linked to CO_2 emissions reduction between CO_2 supplier and CO_2 user in a consistent way and in alignment with external developments, standards and guidelines.	The approach of use of DAC (Direct Air Capture) to partition the benefits between the CO_2 supplier and CO_2 user has practical as well as methodological challenges. With DAC not mature yet, this approach for system expansion credit of CO_2 using systems is quite challenging. Secondly, when DAC process is used with renewable electricity, which is likely the reality of an implementation scenario, the DAC methodological approach does not partition any credits to the CO_2 using system and retains the entire credits of CO_2 capture with the CO_2 supplier thereby compromising the original intent of the approach. Also, external regulations linked to CO_2 capture accounting as well as a reliable certification system may be needed to ensure that CO_2 supplier and CO_2 user will not create potential situations for double-counting of the CO_2 reduction benefits.
2. Caution on use of PCF data based on TfS Guidelines in Comparative assertions on products	Introductory section on Scope of PCF Guidelines (page 37)	Chapter 5.3.3 (page 100)	An additional text that captures a recommendation that PCF calculated using this Guidelines alone can not be used in Comparative assertions on the products.	Since the PCF covers only one of the impact categories that are relevant in an LCA study and the carbon footprint is calculated as Partial PCF (Cradle to Gate), this may miss impacts of carbon footprint arising from other life cycle stages or from other impact categories and thus the Partial PCF may not provide a comprehensive and complete picture for making comparative assertions on such products.

Topic:	"Where to find" in v2.1 and 2.2 document:	"Where to find" in v3 document:	Description of the changes:	Summary of the changes and technical justification driving the change(s):
3. Inclusion process for review and approvals of accepted PCR (Product Category Rules)	Chapter 5.2.4 (page 42)	Chapter 5.2.4.1 (page 52)	Further clarity on the approval process that will be undertaken by TfS Expert Technical Working Group on accepting published Product Category Rules to be listed as "TfS Accepted PCRs).	This is intended to improve the transparency to the process that will be adopted by the Technical Working Group towards amending the Accepted PCRs under TfS Guidelines with every subsequent version of the TfS PCF Guidelines.
4. Definitions of Waste as described under Waste treatment and recycling	Chapter 5.2.8.4 (page 53)	Chapter 5.2.8.4 (page 64)	Formal definitions of Wastes have been included in this section to ensure a definition of waste in alignment with global practices and guidelines.	This clarity establishes a consistent basis on the definition of waste.
5. Descriptions of "Reverse Cut off" and "Cut-off Plus" methods in alignment with formal definitions as per GHG Protocol	Table 5.4 (page 52)	Table 5.4 (page 73)	The reference to "Reverse Cut-off" and "Cut-off Plus" approaches has been revised to standardized definitions of such approaches in alignment with GHG Protocol.	This establishes a consistent description for such allocation, partition or crediting approaches in alignment with taxonomy used by global standards and guidelines such as GHG Protocol.
6. Allocation Hierarchy alignment with Catena-X and WBCSD PACT Guidelines	Chapter 5.2.9 (page 63)	Chapter 5.2.9 (page 76)	Revisions have been made to ensure aligned representation of the text and relevant tables to ensure Allocation hierarchy is in complete alignment with Catena-X and WBCSD PACT.	This revision to the way the Allocation hierarchy is described is needed to ensure consistency and alignment across Industry and Cross-industry Guidelines.
7.Description of Mass balance approach in LCA	Chapter 5.2.10.5 (page 79)	Chapter 5.2.10.5 (page 88)	The procedures of an LCA calculation of mass balance products was introduced including a generic example showing two options of calculation.	This establishes a consistent description for such chain of custody approaches in alignment with current practice and certification schemes.
8. Primary Data share, data quality Rating in alignmnet with Catena-X, GBA and WBCSD PACT	Chapter 5.2.11 (page 79)	Chapter 5.2.11 (page 91)	New assessment systems and caluclation formulas were introduced after harmonization with other standards. Examples were updated.	The revision gives a more in-depth guidance to this important element of assessment and reporting.

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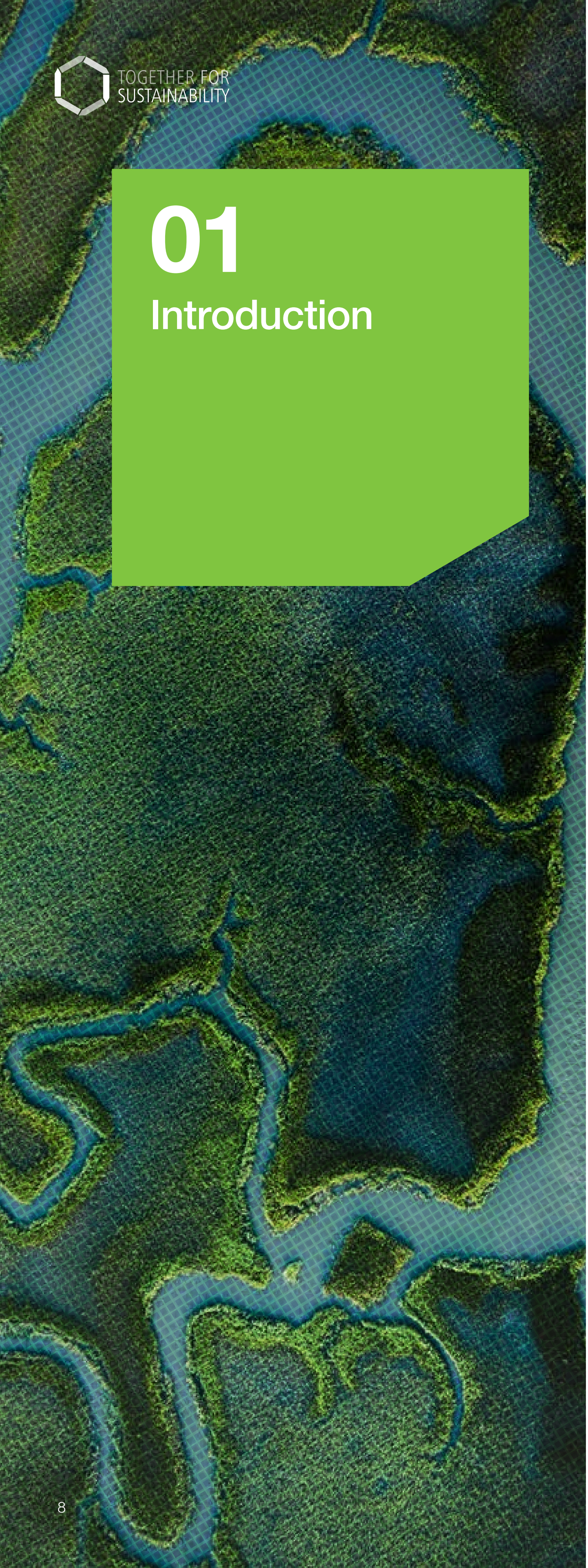

01 Introduction

Anthropogenic GHG emissions drive climate change. The impacts linked to climate change are growing significantly and are a major challenge for the whole world.

To counter this development, the parties of the Paris Agreement agreed on the 1.5°C limit to reduce the effects of climate change and thus avoid irreversible environmental damage and drastic effects for all societies. This requires a high degree of urgency to reduce GHG emissions to a minimum level. Committing to net zero emissions by 2050, latest, is one of the key enablers of this process. The chemical industry contributes 8%[1] to global industrial GHG emissions and thereby must play an important role in reducing GHG emissions.

(1) How to build a more climate-friendly chemical industry | World Economic Forum

Scope 3 emissions are significant for chemical companies. On average, less than one-third of a chemical company's emissions come from the manufacturing of its products, the so-called Scope 1 and 2 emissions. Therefore, for credible corporate carbon accounting and climate target planning and tracking, emissions from the upstream and downstream value chain, or so-called Scope 3 emissions according to the Greenhouse Gas Protocol (GHG P), must be accounted for accurately. Scope 3 emissions are an important part of GHG reduction strategies of all chemical companies and are necessary to understand to prepare for potential future regulations. Particular attention should be paid to the Scope 3 Category 1 "Purchased Goods and Services" emissions (Figure 1.1), which often make up the biggest share of a chemical company's Scope 3, and are thus a key element in its Net Zero strategy.

However, there are many challenges in the reduction of Scope 3 GHG emissions, even for the most committed chemical companies. One challenge is the lack of transparency in value chains, which makes GHG emissions particularly difficult to quantify and reduce. Furthermore, the complexity of the global chemical sector value chain can make it difficult to harmonize calculation approaches and to compare results. Thus comparisons and comparative assertions based on partial PCF (declared unit) for products should be avoided.

Generic standards are a basis for these calculations but are not sufficient due to the lack of specificity for key aspects in the chemical industry. Developing specific guidance on how to address these challenges offers an important opportunity to realize the potential to significantly accelerate the reduction of GHG emissions in the chemical industry (Figure 1.1).

Figure 1.1 TfS PCF Guideline benefits for corporates. Purchased Goods and Services (Scope 3.1) represent a major share of many chemical company's GHG emissions. The TfS PCF Guideline enables corporations to account for Scope 3.1 GHG emissions in a systematic and meaningful way.

DATA AND EFFICIENCY

Learn exactly what chemical PCF data to collect to accurately evaluate Scope 3.1 emissions. Receive comparable data from suppliers for efficient sustainability reporting.

SUSTAINABILITY STRATEGY

Better understand GHG reduction opportunities in your supply chain and create a roadmap to meet sustainability targets.

SUPPLIER SELECTION

Work with suppliers to quantify PCFs in a consistent manner and reduce the footprints of their chemical products.

SUPPLY CHAIN IMPACT

Create a more sustainable supply chain by supporting your suppliers in using the PCF Guideline – as they supply others too.

Collecting and embedding supplier-specific PCFs is beneficial for both 3.1 and PCF accounting (Figure 1.2). Annual corporate-level 3.1 emissions can be improved by applying PCFs of high quality provided by suppliers for purchased goods, allowing companies to track progress over time towards climate goals. Additionally, by integrating supplier-specific PCFs within corporate 3.1 inventories, GHG emissions associated with the specific raw materials can be linked to production processes of chemical companies, improving the accuracy of their PCFs. In many cases, a chemical company is both a supplier and a manufacturer; therefore, from a chemical industry perspective, it is extremely important to calculate PCFs of high quality and high level of comparability. Furthermore, supplier PCFs can also be used to identify reduction potentials within the company's purchasing department in the form of product portfolio adjustments and collaborations with suppliers to decarbonize.

Therefore, a basic condition for the implementation of PCFs to 3.1 accounting is a harmonized approach that shows how PCFs should be calculated considering all specific aspects of chemical production processes. The methodological approach has an important impact on the results and their quality, which makes it important for companies to collect accurate and comparable data as well. Likewise, there is a need for a consistent solution or standard on how to share PCF data.

Figure 1.2 Benefits for chemical suppliers by applying the TfS PCF Guideline. Chemical suppliers can provide accurate and consistent PCFs to corporate customers to support them in accurately reporting and reducing their Scope 3 category 1 emissions.

Better understand the GHG emissions associated with your products – so you can **improve sustainability performance and reporting and reach emissions-reduction targets**.

Improve efficiency, streamline resources and **reduce the amount of time you spend using generic guidelines**.

Report PCFs to the level of specificity many customers are requesting – so you can **increase customer satisfaction and generate new sales**.

This guideline aims to provide instructions for the calculation and implementation to the subsequent reporting of Scope 3.1 emissions, with the goal of creating transparency within the supply chain and comparability across the chemical sector. The underlying calculation of PCFs as the basis for Scope 3.1 reporting is provided and recommendations are made on how to share the PCFs including additional information (data attributes).

This Guideline is the first-of-its-kind, industry-specific guidance on calculating PCFs for chemical products empowering companies to produce high quality PCF data. It is compliant with ISO 14067 and GHG Protocol accounting standards.

02
About the Guideline

2.1 Background and context

The global chemical sector initiative TfS, has developed a global open-source sector-specific guideline for the calculation of PCF and Scope 3.1 reporting. It can be applied in the chemical industry and beyond. It treats several challenges as follows:

- Scope 3 emissions of purchased goods have historically been challenging to measure due to the complexity of chemical production – the new Guideline aims to solve this.
- The Guideline can be used by both corporations and suppliers to identify, track, and reduce Scope 3 upstream emissions.
- The Guideline will be applicable across industries; it will be open source and useful for other industries using chemical materials.
- It harmonizes PCF calculation approaches across the industry and is applicable to most chemical products. In the future, this will allow consumers and the wider market to directly compare and assess the climate impact of products. Practitioners should evaluate if the Guideline is applicable to their specific products, and justify if not.

The TfS initiative developed this guideline to take a leading role in a more sustainable chemical industry by providing guidance in calculating PCFs and Scope 3 emissions. The development was done by a group of experts from TfS member companies, supported by external experts, reviewed by more than 55 companies within the chemical sector and audited by TÜV Rheinland. Existing standards and guidelines were considered and used as a basis for creating sector-specific text for the chemical industry. [WBCSD (2013), ICCA & WBCSD (2013)].

In the past, the calculation and reporting of Scope 3 GHG emissions have differed between companies in the chemical sector due to the range of possible choices when following the internationally recognized GHG standards. This document has been developed to introduce a consistent guideline which companies from the chemical sector can follow when calculating Product Carbon Footprints (PCF) or emissions resulting from Purchased Goods and Services (Scope 3.1). [WBCSD (2013), ICCA & WBCSD (2013), WBCSD (2014)].

Following this guideline will allow the TfS member companies and their suppliers to align in their GHG accounting and reporting. By introducing a consistent reporting standard, the comparability between chemical companies can be improved, which benefits the company, clients, investors, and other external stakeholders during performance assessments.

If multiple chemical companies transparently disclose their emissions and sustainability measures following the same standards, internal business decisions at each company can be improved and the overall role of chemical products in reducing GHG emissions can be communicated more effectively to internal and external stakeholders or business partners. Furthermore, TfS aims to inspire other industries facing similar problems to improve their respective reporting standards.

2.2 Governance process for periodic review of the present guideline

This document is the third version of the PCF Guideline that TfS has created to support chemical companies in improving their calculation and reporting of product carbon footprints and emissions resulting from Purchased Goods and Services (Scope 3.1). TfS is aware that the current version of this guideline can and should be further developed in the future as standards and other underlying documents might change. Participating companies and other stakeholders can continuously report back about possible additions and adjustments which will then be considered during the guideline updates. Furthermore, TfS plans to periodically harmonize the guidelines with new developments in internationally recognized standards, such as ISOs, or other related guideline documents.

2.3 Problem statement

General problems described in chapter 2.1 are to be dealt with and described in more detail here. A relevance analysis of gaps in standards supported the development and integration of new text. Which of the missing elements are significantly relevant for the chemical industry and Scope 3.1? Do we need to go deeper at certain points? If yes, where?

Addressing issues and requirements, e.g.:

- The boundary of a cradle-to-gate life cycle inventory shall not include product use or end-of-life processes.
- The scope of the guideline covers cradle-to-gate calculations for chemicals. The gate is defined as the gate of TfS members.
- Guidance on how to categorize, evaluate and use data sources, be it from primary or secondary data sources.

Calculation rules for specific products including the treatment of biomass, biomass balanced materials, recycled materials, system expansion, allocation schemes, cut off rules, system boundaries are important aspects and methodological elements that will be considered.

2.4 Objective of the guideline

2.4.1 Design of a consistent process for Scope 3.1 data collection

- Describe boundaries and principles for Scope 3.1 data collection for material product categories.
- Develop a uniform process for data collection and emission calculation.
- Establish a robust/audit proof guideline which can be applied by all TfS member companies.
- Harmonized and sector-specific guideline for PCF calculation.

2.4.2 Embedding supplier PCF data in downstream PCF calculations

The application of chemicals is an additional topic and is covered in some specific GHG Protocol categories. PCF figures of high quality are needed to calculate meaningful cradle-to-grave applications. The guideline supports indirectly the reporting in these categories but this is not in focus here. However, using recycling materials or bio-based materials from downstream applications as raw materials for chemicals are considered here as well.

2.5 Importance of content considered

Many organizations have now started to develop guidelines and supporting materials to enable companies to report their GHG emissions in a harmonized and accepted environment. In this guideline, chemical sector-specific guideline is given to increase transparency and increase harmonization in the sector. This guideline aims to set standards for a more consistent accounting of Scope 3.1 (Purchased Goods and Services) emissions and the assessment of product carbon footprints (PCFs) in the chemical sector. It is intended to be used by companies in the chemical industry that want to improve on these aspects of their carbon footprint reporting.

In 2013, the World Business Council for Sustainable Development (WBCSD) published a “Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain”, in which they identified Scope 3.1 emissions to be the most relevant Scope 3 category for chemical companies, due to both the large size of expected emissions and the amount of influence companies have on the category (see Figure 2.1). For this reason, TfS decided to put the first focus of this guideline on creating consistent guidelines for the accounting of Scope 3.1 emissions in chemical companies. [WBCSD (2013), GHG Protocol Corporate Value Chain Standard (Figure 2.1)].

Figure 2.1 Relevant categories of Scope 3 emissions for chemical companies.
(Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain, WBCSD, 2013)

Expected size of emissions (relative to company total)	Influence on emissions in the category: Large			Small
Small			6. Business travel 7. Employee commuting	13. Downstream leased assets 14. Franchises 15. (Financial, debt, bonds, pension funds & other) Investments
Medium	2. Capital goods 3. Fuel- and energy-related activities 4. Upstream and purchased transportation & distribution	8. Upstream leased assets 15. (Material equity) investments	5. Waste generated in operations 9. Downstream transportation & distribution	10. Processing of sold products
Large	1. Purchased goods & services	12. End-of-life treatment of sold products	11. Direct emissions from use of sold products	11. Indirect emissions from use of sold products

The second part of this guideline focuses on specifications for embedding supplier PCF data into downstream customer's PCF calculations. Since chemical products are often further processed, PCFs of these products are crucial to calculate the chemical industry's contribution to the PCF of products in other industries and applications. The PCF figures are reported by the companies purchasing these products in category 3.1 in corporate accounting.

Both, standardized methods for Scope 3.1 inventories and PCF calculations will help chemical companies and their customers to credibly communicate potential GHG impacts and strategies to reduce the associated risks along the value chain. Moreover, with demand for environmentally conscious products and services growing, credible information on PCFs and Scope 3.1 emissions will become substantial for internal decision processes about future product and market strategies [WBCSD (2014)].

2.6 Methodology and reference to existing standards and guiding documents

The guidelines in this document aim to be consistent with internationally accepted standards and requirements. The following standards were considered:

- ISO 14064 -1: 2019
- ISO 14067: 2019
- ISO 14040:2006/Amd 1:2020
- ISO 14044:2006/Amd 2:2020

The guideline follows these standards:

- GHG Protocol Corporate Value Chain (Scope 3).
- GHG Protocol Scope 3 Calculation Guidance.
- GHG Protocol Product Standard.

Additionally, various other documents have been reviewed to harmonize the structure and logic of the approach of this document. These documents are listed in the reference list accordingly. The guideline can be used as drop-in solution for other sectors and sector-specific guidelines that are using chemicals in their products. As such, some chapters and text might be useful to be integrated in other sector-specific guidelines as well.

The main part of this guideline is divided into three parts.

Chapter 3 introduces the five principles of GHG accounting, which help to guide the implementation of the GHG Protocol Standards.

Chapter 4 addresses the assessment of Scope 3.1 emissions. It provides input about the processing of Activity Data (Chapter 4.3), the selection and evaluation of Emission Factors (Chapter 4.4), Input Data Processing (Chapter 4.4), the Target Baseline recalculation (Chapter 4.5), and Additional accounting and reporting guidelines (Chapter 4.6).

In **Chapter 5**, specifications for suppliers' product carbon footprint calculations are given. After introducing the general goal and scope of a PCF (Chapter 5.1), the calculation rules (Chapter 5.2) are introduced. Chapter 5.3 finishes with information about the verification of PCF calculations and notes about the reporting of PCFs. [WBCSD (2023), European Commission (2021)].

2.7 Terminology: shall, should, and may

This standard uses precise language to indicate which provisions of the standard are requirements, which are recommendations, and which are permissible or allowable options that companies may choose to follow. The term "shall" is used throughout this standard to indicate what is required in order for a GHG inventory to be in conformance with the GHG Protocol Scope 3 Standard. 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].

This standard uses precise language to differentiate between the levels of obligation a company faces when following the proposed guidelines. As defined by ISO International Standard:

- "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."[1]

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03 Reporting Principles

GHG accounting and reporting of a Scope 3 or a product inventory shall be based on the following principles:

Relevance, Completeness, Consistency, Transparency, and Accuracy. [World Resources Institute and WBSCD (2004)].

The primary function of these five principles is to guide the implementation of the GHG Protocol Standards and the assurance of the inventories, particularly when application of the standards in specific situations is ambiguous. The same principles are also used to access the uncertainty within reported data.

In practice, companies may encounter trade-offs between principles. For instance, a company may find that achieving the most complete inventory relies on less precise data, compromising overall accuracy. Conversely, achieving the most accurate inventory may require excluding activities with low accuracy, compromising overall completeness. Companies should balance trade-offs between principles depending on their individual business goals. Over time, as the accuracy and completeness of Scope 3 and PCF GHG data increases, the trade-off between these accounting principles will likely decrease.

Each principle is briefly described below, with more information provided in chapter 4.

Relevance

A relevant Scope 3.1 report contains the information that users – both internal and external to the company – need for their decision making. Companies should use the principle of relevance when determining whether to exclude any activities from the inventory boundary, selecting data sources, and collecting data.

Completeness

Companies should ensure that the inventory appropriately reflects the Scope 3.1 GHG emissions of the company. In some situations, companies may be unable to accurately estimate emissions due to a lack of data or other limiting factors. However, companies should not exclude any emissions sources that would compromise the relevance of the reported inventory. Any exclusions should be transparently documented and justified; assurance providers can determine the potential impact and relevance of the exclusion on the overall report.

Consistency

The consistent application of accounting approaches, inventory boundary, and calculation methodologies is essential to producing comparable GHG emissions data over time. If there are changes to the inventory boundary (e.g., inclusion of previously excluded activities), methods, data, or other factors affecting emission estimates, they need to be transparently documented and justified, and may warrant recalculation of base year emissions.

Transparency

Transparency relates to the degree to which information on the processes, procedures, assumptions and limitations of the GHG inventory are disclosed in a clear, factual, neutral, and understandable manner based on clear documentation. A transparent report will provide a clear understanding of the relevant issues and a meaningful assessment of emissions performance of the company's Scope 3 emissions. Information should be recorded, compiled, and analyzed in a way that enables internal reviewers and external assurance providers to attest to its credibility and to derive the same results if provided with the underlying data sources.

Accuracy

Data should be sufficiently accurate to enable intended users to make decisions with reasonable confidence that the reported information is credible. GHG measurements, estimates, or calculations should neither be systemically over nor under the actual emissions value, as far as can be judged[1]. Companies should reduce uncertainties in the quantification process as far as practicable and ensure the data are sufficiently accurate to serve decision-making needs. Reporting on measures taken to ensure accuracy and improve accuracy over time can help promote credibility and enhance transparency.

(1) In the case of mass balance, conventional (non-mass balanced) products are affected by the dedicated use of sustainable feedstocks for the mass-balanced products. In that sense, the actual mixture of feedstocks is not considered in the PCF of the non-mass balanced products in order to ensure that no double-counting occurs and the CO_2 balance is closed.

04
Guidance on Scope 3.1 Calculation on Corporate Level

The product system of the cradle-to-gate PCF is the sum of GHG emissions, expressed as CO_2 equivalents related to a product, from the extraction of the resources to the gate of the reporting company including transportation.

The PCF calculation may include the transportation to the customer, but the respective GHG emissions must be stated as additional information separately from the cradle-to-gate PCF.

The PCF of chemicals shall include all product related GHG emissions. How to calculate PCF for chemicals is described in detail in chapter 5 of this document.

In the context of corporate reporting, PCFs are used to calculate Scope 3.1 emissions. GHG emissions of a reporting company are divided into three Scopes as defined by the Greenhouse Gas Protocol (GHG Protocol):

Scope 1 direct CO_2e emissions result from the production processes that are owned or controlled by the reporting company. For example, direct emissions from chemical reactions, incineration, or waste treatment at the reporting company's plant or emissions from the production of on-site energy.

Scope 2 CO_2e emissions result from the generation of purchased energy, such as electricity and steam used to power the reporting company's plants.

Scope 3 CO_2e emissions occur from sources owned or controlled by other entities in the value chain. Within Scope 3, there are 15 sub-categories [GHG Protocol Corporate Value Chain (Scope 3) Standard] that cover the emissions from the upstream and downstream value chain. This guideline focuses on Scope 3.1, Purchased Goods and Services, with a primary focus on purchased goods. While their emissions may be relevant, other Scope 3 categories are not considered herein; chemical companies should assess the relevance of these categories and their impact on their PCFs. If upstream transportation is not included as part of scope 3.1 then it shall be reported as part of scope 3.4, which is outside the scope of this document.

For chemical companies, the most emissions-intense purchased goods are often raw materials used and transformed to products. For annual corporate reporting, the PCF values of each purchased good are aggregated to one value and are reported in the category Scope 3.1. Based on the PCF information for those purchased goods, companies calculate the PCF for their end products to achieve a cradle-to-gate result. The resulting PCF is the calculation basis for the next producer in the supply chain.

4.1 Definition of Scope 3.1 Purchased Goods and Services

According to the Greenhouse Gas Protocol [GHG Protocol Corporate Value Chain (Scope 3) Standard] this category includes all upstream (i.e., cradle-to-gate) emissions of products purchased or acquired by the reporting company. Products include both goods (tangible products) and services (intangible products). This category includes emissions from all Purchased Goods and Services not otherwise included in the other categories of upstream Scope 3 emissions (i.e., category 2 through category 8).

Cradle-to-gate emissions include all emissions that occur in the life cycle of purchased products, up to the point of receipt by the reporting company (excluding emissions from sources that are owned or controlled by the reporting company). Cradle-to-gate emissions may include:

- Extraction of raw materials.
- Agricultural activities.
- Manufacturing, production, and processing.
- Generation of electricity consumed by upstream activities.
- Packaging and other auxiliary materials (as e.g. filter aid).
- Disposal/treatment of waste generated by upstream activities.
- Land use and land-use change.
- Transportation within the upstream supply chain and to the reporting company, when not paid for by the reporting company.
- Any other activities prior to acquisition by the reporting company.

Chapter 5 describes how cradle-to-gate PCF shall be calculated. For the chemical industry Scope 3.1. materials are very important, because relatively high contributions to the overall PCF are caused in the early steps of raw material generation. Companies using PCF information from their suppliers to implement them in Scope 3.1 upstream reporting should check if:

- The data provided by suppliers is of an acceptable age as described in 5.2.2 and not outdated.
- The declared unit fits exactly to the form the company is using the product.
- The quality and the concentration fit to the used product.
- The data quality is sufficient to be used in the reporting.
- The variation between several suppliers is plausible and supported by evidence.
- The attributes delivered with the PCF of the product should be complete and representative for the product.

4.2 Foundations of the 3.1 accounting process

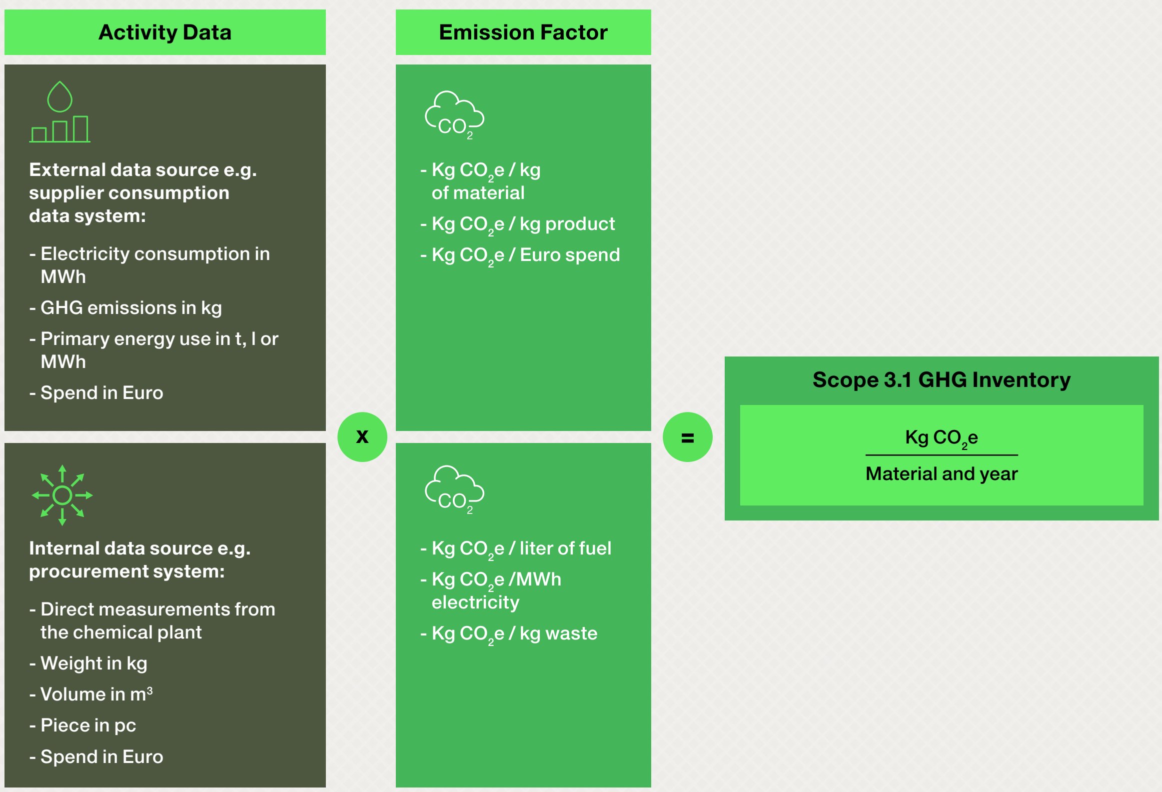
This section covers the best practices for building a GHG inventory and GHG emissions calculation techniques. A GHG inventory accounts for all GHGs emitted to or removed from the atmosphere by the reporting company. The GHG inventory will list, by source or GHG Scopes, the amount of GHG emissions emitted to the atmosphere during a given time period (mostly within the time of a company's reporting cycle). Particular attention needs to be paid to the selection of the inventory boundary. The boundary needs to balance completeness and consistency with the relevance of Scope 3.1 emissions. Chapter 3 of The Greenhouse Gas Protocol provides detailed instructions on best practices for setting inventory boundaries. [WBCSD Chemicals, (2013)]

To build a Scope 3.1 GHG inventory, inventory boundaries, data basis, and methodologies need to be consistent to allow meaningful conclusions and performance tracking over time. Hence, the inventory boundaries and the data sources for activity data, as well as emission factors, need to be carefully selected. That said, continuous improvement in data quality should be strived for to enable emissions to be characterized in the most accurate way. Any changes from previous years may affect a company's Scope 3 GHG inventory and should therefore be undertaken only with careful consideration of the significance of the activity and the expected benefit from the increased data quality. However, to ensure comparability over time, a change in the calculation practices should be transparently reported and could necessitate the recalculation of the base year emissions. In chapter 4.4 various approaches to reduce effort and complexity without overly compromising quality are provided.

The emissions inside a GHG inventory are quantified using either direct measurement or calculation methods. As direct measurement data for Scope 3 emissions are difficult to obtain for the reporting company, usually such information is estimated using calculation methods, making use of activity data and emission factors. According to the GHG Protocol, “activity data” is a quantitative measure of a level of activity that results in GHG emissions (for example, kilograms of purchased material or dollars spend on an activity). An “emission factor” is a factor that converts activity data into GHG emissions (for example, kg CO_2 emitted per kilogram or dollar spent). Figure 4.1 gives an overview of the elements of Scope 3.1 GHG inventory data, and activity data generation (chapter 4.4) and emission factor collection (chapter 4.5) are described in detail in the following sections.

The GHG Protocol differentiates GHG calculations into four basic methods: Spend, Average, Hybrid and Supplier method [GHG Protocol Scope 3 Calculation Guidance (2013)]. The methods can differ significantly in the way data are collected and processed resulting in significant differences in effort and accuracy. Although it might be partially unpractical or can create additional effort, methodologies can be used in combination. The decision for or against a specific method can depend on a company’s business goals, the significance of goods and services emissions within Scope 3.1, and the availability and quantity of data, if data quality allows, supplier-specific values are always preferred.

Figure 4.1 General calculation approach of preparing an GHG inventory



4.3 Activity data

Activity data used for calculating Scope 3.1 emissions are typically the quantities of procured raw materials and/or monetary spend on services or technical goods purchased in the reporting year.

4.3.1 Activity data collection and processing

Activity data is a key input for the calculation of GHG emissions and refers to the data associated with an activity that generates GHG emissions, such as tons of a raw material purchased. This activity data is collected in physical units (tons) or money spent and then combined with an emissions factor and the relevant greenhouse gas GWP value to calculate CO_2e. The collection of activity data is the primary responsibility of the reporting company and will often be the most significant challenge when developing a GHG inventory. Therefore, establishing robust activity data collection procedures is essential. Companies may find it useful to differentiate between purchases of production-related and non-production-related products. Doing so may be aligned with existing procurement practices and therefore may be a useful way to organize and collect data more efficiently.

Production-related procurement (often called direct procurement) consists of purchased goods that are directly related to the production of a company's products. Production-related procurement may include:

- Raw materials and intermediate goods (e.g., materials, components, and parts) that the company purchases to process, transform, or include in another product.
- Final goods purchased for resale (for retail and distribution companies only).
- Technical and capital goods (e.g., plant, property, and equipment) that the company uses to manufacture a product, provide a service, or sell, store, and deliver merchandise or that need to be purchased as well to enable the chemicals and accurate application of the products by the customer. Examples of technical and capital goods within the chemicals industry include packaging, water cleaning chemicals, or chemicals used in cooling towers, etc.

Note that capital goods are reported in Scope 3 category 2 (Capital Goods).

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 furniture, office equipment, and computers or all kinds of services such as consulting, maintenance work, or contracted labor.
[GHG Protocol Corporate Value Chain (Scope 3) Standard]

The processes of activity data generation, preparation and handling are summarized in Figure 4.2 and described in detail below.

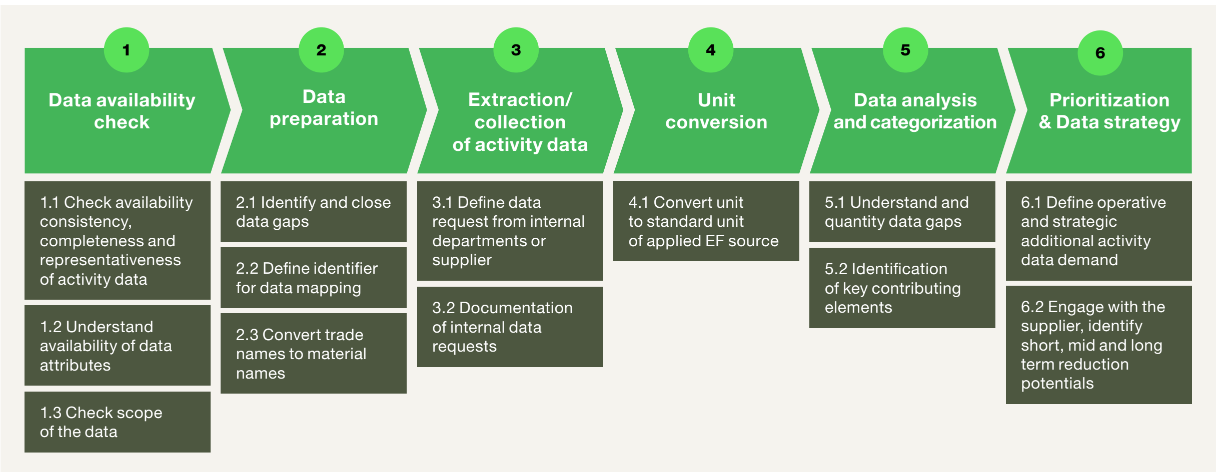
Data availability check

1.1) Activity data may be obtained through meter readings, purchase records, direct monitoring, mass balance, stoichiometry, or other methods, for obtaining data from specific activities in the company's value chain see also text in 5.2.5 and 5.2.8. Activity data could be taken from internal procurement and/or ERP systems or requested from the supplier directly.

Data on spend and mass, volume, quantities of products shall be internally requested. In addition, an understanding of the internal systems their update frequencies, units, formats, availability of forecasting values, potential changes should be generated and implications on the intended accounting system anticipated. The availability of the data within the annual accounting cycle should also be considered to ensure that data are available at the right time and in the right quality for further calculations.

1.2) Besides the actual activity data numbers, the attributes of the purchased goods are needed. Primary attributes refer to the material directly (e.g., material name, number, CAS, chemical structure, chemical group), while secondary attributes further specify indirect characteristics (e.g. year, vendor country, supplier name, supplier number). These attributes allow for the mapping

Figure 4.2 Key process steps of Scope 3.1 activity data generation, preparation, and handling



of activity data to emission factors and the analysis and interpretation of the data.

1.3) In a last verification step, the data extracted from the internal system should be checked to ensure that it is accurate and consistent. These checks can be conducted internally and do not require external verification.

Preparing for data collection

2.1) While spend data might be of good completeness due to requirements from financial accounting, physical data on the amount, volume, or mass of purchased goods might be incomplete and/ or inconsistent. Because usually dozens or even hundreds of persons are involved in the companies purchasing process, a change in the process of the data collection might have larger implications on the processes and systems. Having a complete set of physical input data might be a long-term challenge for many, it is recommended to start the data preparation step as soon as possible.

2.2) The potentially large amount of data that need to be handled, the heterogeneity and even unavailability of material numbers as well as the use of various internal and external data sources can make it necessary to establish a proper data management system that goes beyond widely used Excel-based systems. In both cases the use of an identifier is essential to guarantee traceability and uniqueness of data base entries. A list of identifiers already used in the chemical sector is provided in Table 4.1, in which the Chemical Abstract Service (CAS) is the most widely accepted and used system at chemical companies but also at providers of emission factor data. Companies may develop their own identifiers for purchased goods or services outside the chemical classification systems, e.g. packaging, labor services, or IT products.

Table 4.1 Examples of classification systems that could be used as identifier in the mapping process of activity data and emission factors

Abbreviation	
Chemical Abstracts Service Registry (CAS) Number	A CAS Registry Number 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[1].
Simplified Molecular Input Line Entry System (SMILES)	The simplified molecular-input line-entry system is a specification in the form of a line notation for describing the structure of chemical species using short ASCII strings[2].
ECLASS	ECLASS is a worldwide ISO/IEC-compliant data standard for goods and services[3].
United Nations Standard Products and Services Code (UNSPSC)	The United Nations Standard Products and Services Code is a global classification system of products and services. These codes are used to classify products and services: in the case of suppliers, to classify the products and services of their company, and in the case of UN staff members, to classify the products and services when publishing procurement opportunities[4].
PRODCOM	PRODCOM is an annual survey for the collection and dissemination of statistics on the production of industrial (mainly manufactured) goods, both in value and quantity terms, in the European Union (EU)[5].
European Customs Inventory of Chemical Substances (ECICS)	The European Customs Inventory of Chemical Substances is an information tool managed by the European Commission's Directorate General (DG) for Taxation and Customs Union which allows users to: - Clearly and easily identify chemicals; - Classify them correctly and easily in the Combined Nomenclature; - Name them in all EU languages for regulation purposes[6].
Harmonized Commodity Description and Coding Systems (HS)	The Harmonized System is an international nomenclature for the classification of products. It allows participating countries to classify traded goods on a common basis for customs purposes. At the international level, the Harmonized System (HS) for classifying goods is a six-digit code system[7].

(1) https://www.cas.org/cas-data/cas-registry
(2) https://www.chemeurope.com/en/encyclopedia/Simplified_molecular_input_line_entry_specification.html
(3) https://www.eclass.eu/en/index.html
(4) https://www.unspsc.org/
(5) https://ec.europa.eu/eurostat/statistics-explained/index.php?title=Glossary:PRODCOM
(6) https://ec.europa.eu/taxation_customs/online-services/online-services-and-databases-customs/ecics-european-customs-inventory-chemical_en
(7) https://unstats.un.org/unsd/tradekb/Knowledgebase/50018/Harmonized-Commodity-Description-and-Coding-Systems-HS

2.3) For further processing and mapping procedures it might be helpful to convert the trade names as defined by the supplier to standardized material names. If such effort is needed depends on the quality of the procurement databases but also on the applied strategy to map activity data with emission factors. For example, an automated mapping based on CAS numbers doesn't need uniquely defined material names. A mapping strategy that manually maps emission factors and activity data based on material names would require a clean and unique material name.

Extraction/collection of activity data

3.1) The extraction of activity data from internal systems or the collection from the supplier should start with the distinct definition of the data request. Beside the material specific definitions (compare typical data attributes) it should have general information on available data and file formats.

- Date of data extract.
- Data system used & version.
- Relevant data points (PCF/Inventory data mass, volumes, energy, etc.).
- Timeframe (e.g., reference period).
- Geographical boundary (country).
- Technological boundary (e.g., material or production specifications (concentration)).
- Company scope (e.g., operational boundaries).
- Unit.
- Further data attributes (Pro Taxonomy, supplier name, Dun & Bradstreet (DUNS) number).

3.2) The processing of external and internal data requests makes it necessary to extract data from the reporting companies' procurement or ERP systems. Database extractions (e.g., queries) should be documented and saved to guarantee comparability and consistency over time but also to provide confidence in the verification process of the assurance company.

Unit conversion

4.1) Clearly defined activity data might also be delivered with different units, or units that do not correspond to the units applied in the emission factor datasets. While a unit conversion from different measuring units (metric/imperial) or monetary units might be easy to handle with standardized factors, a conversion between different physical units (volume – mass or piece – mass) needs product- or material-specific factors. Average factors on density, for example, might help in most of the cases, however the applicability to specific products should be carefully checked. The same holds true for conversions from piece-based units to mass-based units.

Data analysis and categorization

5.1) The analysis step should help the reporting company to make decisions with respect to further processing and improving of the data, based on data completeness and quality. In a first step, the reporting company should understand which activity data points are available for the different types of data (physical, spend based). In a second step, the extent of existing data gaps needs to be estimated to support the definition of a data strategy.

5.2) A hot spot analysis based on physical or spend data might help to identify key suppliers as well as goods and services that contribute the most to the inventory. A categorization of goods and services with similar properties might then help to close the data gaps identified in 5.1.

Prioritization and data strategy

6.1) Based on the data analysis, high priority areas per supplier, goods, and service category as well as further data demand might be identified. The operative and strategic data demand should be defined in a data strategy as well as approaches, processes, and systems to close those gaps.

6.2) It is unlikely that all suppliers of a reporting company will be able to provide PCF data. In such cases, companies should encourage suppliers to develop GHG inventories. If GHG emission data from suppliers is not available, emission factors from other sources should be used (please see chapter 4.4 emission factors).

4.3.2 Clustering and prioritization of activity data

The prioritization of Purchased Goods and Services is an important step in 3.1 activity data assessment. It can be done by following a two-step approach.

Step 1: Clustering

For a chemical company with thousands of Purchased Goods and Services, clustering the company's own purchases into product groups can facilitate calculation [Global Compact Network Germany (2019)]. For purchased goods, is recommended to cluster purchases according to their profile (e.g., CAS number), considering the level of aggregation of available emission factors. For a better overview and data processing, clustering can be useful at e.g., procurement category, sub-category or material group level. This facilitates the selection of emission factors e.g., from LCA databases and allows, if applicable, an extrapolation of GHG emissions to account for 100% of the raw materials purchased within a category of (chemically) related substances (please see 4.4 extrapolation). This approach can improve the accuracy of such an extrapolation step.

For non-raw material related purchased goods & services, spend data can be used to cluster goods. Classifying by international accepted sector groups (e.g., NACE codes) may be useful, using the coverage and rationale used for clustering sectors and regions within environmentally-extended input (EEIO) output data[1] tables and models as a guide, such as Exiobase or the 2014 guidelines to Defra / DECC's GHG Conversion Factors for Company Reporting (Table 13 - Indirect emissions from the supply chain). This publicly available document provides spend-based emission factors for over 100 product groups or sectors according to the standard industrial classification.

(1) Environmentally-extended input output (EEIO) models estimate energy use and/or GHG emissions resulting from the production and upstream supply chain activities of different sectors and products within an economy. The resulting EEIO emissions factors can be used to estimate GHG emissions for a given industry or product category. EEIO data are particularly useful in screening emission sources when prioritizing data collection efforts. EEIO models are derived by allocating national GHG emissions to groups of finished products based on economic flows between industry sectors. EEIO models vary in the number of sectors and products included and how often they are updated. EEIO data are often comprehensive, but the level of granularity is relatively low compared to other sources of data.

Step 2: Prioritization

Prioritizing activities based on the magnitude of GHG emissions

The most rigorous approach to identifying priority activities is to use initial GHG estimation (or screening) methods to determine which Scope 3.1 goods or services are expected to be most significant in size based on factors like purchased weight or spend. A quantitative approach gives the most accurate understanding of the relative magnitudes of various Scope 3.1 activities.
To prioritize activities based on their expected GHG emissions, companies should:

- Use initial GHG estimation (or screening) methods to estimate the emissions from each Scope 3.1 activity (e.g., by using industry-average data, EEIO data, proxy data, or rough estimates);
- Rank all Scope 3.1 goods or services from largest to smallest according to their estimated GHG emissions to determine which Scope 3.1 activities have the most significant impact; and
- Apply the guidance in Chapters 5.2.6 until 5.2.8 of this document.

Companies should also assess whether any GHG- or energy-intensive materials or activities appear in the value chain of purchased goods, e.g. precious metals based materials such as catalysts.
[GHG Protocol Corporate Value Chain (Scope 3) Standard].

Companies may find it useful to differentiate between purchases of production-related products (e.g., materials, components, and parts) and non-production-related products (e.g., office furniture, office supplies, and IT support). This distinction may be aligned with procurement practices and therefore may be a useful way to organize and collect data more efficiently and showing the contributions to the overall emissions of Scope 3.1 (Figure 4.3).

Figure 4.3 An example of impacts to Scope 3.1 reporting of different raw materials according to their share of contribution

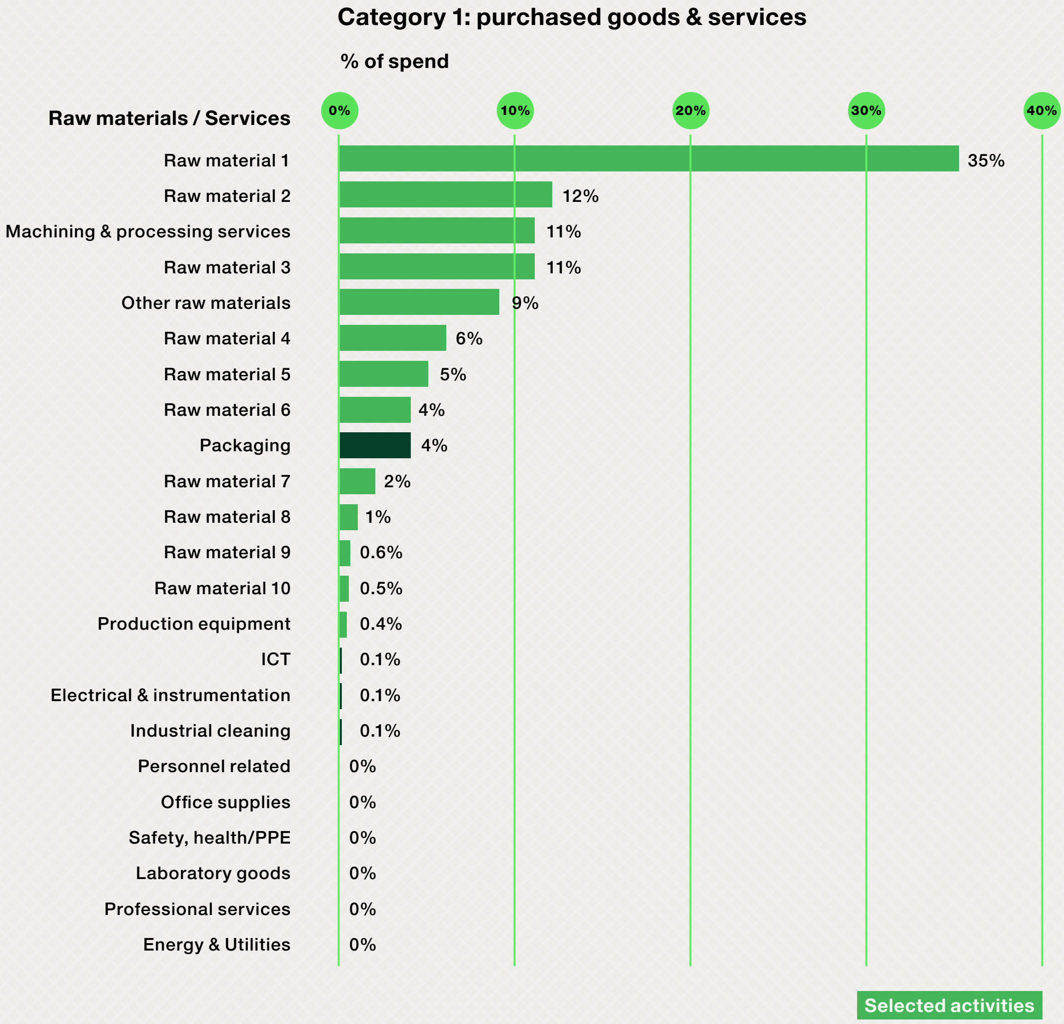


Table 4.2 Prioritization of Purchased Goods and Services based on CO_2 vs spend. Following the 80/20 rule, using top 80% of CO_2 emissions prioritizes only raw materials, whereas using 80% of spend prioritizes both raw materials and services.

Purchased good or service	% of estimated CO_2	% of spend
Raw material 1	35%	20%
Raw material 2	20%	15%
Raw material 3	10%	10%
Raw material 4	15%	5%
Raw material 5	5%	5%
Information technology	3%	5%
Financial services	5%	5%
Labor services	5%	15%
Consulting services	2%	20%

The spend-based method is the least accurate method, as spend relies on financial impacts, such as inflation, taxes & currency effects.

Prioritizing activities based on financial spend or revenue

If a ranking of Scope 3.1 activities based on their estimated greenhouse gas emissions is not possible, companies may choose to prioritize Scope 3.1 activities based on their relative financial significance. Companies may use a financial spend analysis to rank upstream types of purchased products by their contribution to the company's total spend or expenditure (for an example, see the company case study on the right-hand side).

Companies should use caution in prioritizing activities based on financial contribution, because spend and revenue may not correlate well with emissions. For example, some activities, like financial services, have a high market value, but have relatively low emissions. Conversely, some activities have a low market value, but have relatively high emissions, such as some raw materials. As a result, companies should also prioritize activities that do not contribute significantly to financial spend or revenue but are expected to have a significant GHG impact.

It should be noted that the emission factors of the 2014 guidelines to Defra/DECC's GHG Conversion Factors for Company Reporting were only maintained up to 2011 and are related to British Pounds 2011 (incl. VAT). These emission factors must be adjusted to the currency inflation rate in the current reporting year, the relevant exchange rate and VAT, before applying them.

Example from GHG Protocol: Prioritizing Scope 3 emissions from Purchased Goods and Services

A specialty chemicals company conducted an emission and spend-based analysis to prioritize its Purchased Goods and Services before collecting data for category Scope 3.1. The company set out to identify the Purchased Goods and Services that together accounted for at least 80% of emissions and 80% of total spend. Table 4.2 shows how the results of the prioritization differ when expenditures are considered instead of GHGs. In particular, the inclusion of high expenditure leads to large differences.

4.3.3 Activity data updates & improvement

Each year, the reporting company shall update the amounts of Purchased Goods and Services. The company shall also account for any new categories and types of purchases. Any material errors identified that would impact previous year calculations are to be corrected for current year and prior year calculations, as described in more detail in the GHG Protocol [GHG Protocol Corporate Value Chain (Scope 3) Standard]. Over time, more accurate data sources may be identified. These are also to be applied to current year and previous year calculations, except for such case where the new data source is found not relevant for a previous year.

The applied data collection methodology shall be maintained each year to appropriately make comparisons and track progress. However, a company may find over time that purchases need to be in a different Scope 3 category than originally assumed. While this is not a material change in Scope 3 emissions for the company, it does reflect an opportunity to improve data accounting accuracy. This type of change could trigger a recalculation of the base year emissions, in order to maintain consistent comparisons.

4.4 Emission factors

As previously discussed, emissions can be quantified using direct measurements or calculations, though Scope 3 emissions most commonly employ a calculation approach using activity data and emission factors.

Calculating Scope 3 emissions based on emission factors can lead to large variations and uncertainties, thus, the availability of suitable emission factors is a key factor for the quality of the Scope 3.1 GHG inventory. The following steps provide guidance on best practices to finding and using emission factors (Figure 4.4).

1) Data availability check and emission factor strategy

Emissions factor can be taken from various sources, in different qualities and different scopes. An overview of different data types is given in Table 4.3. When taking emission factors from databases, these shall be always sourced from verified databases. Examples of emission factors sources are as follows:

- Verified data from associations that are compliant with ISO 14067.
- LCA databases such as Sphera Managed LCA content (MLC), Ecoinvent, Carbon Minds, Agribalyse, ELCD (PEF) database.
- Official national emission factor databases such as US EPA, IEA, Defra (e.g., DECC for spend-based data), etc.
- Supplier data.

2) Data extraction

A company internal prioritization is needed on which data shall be used to track the emissions from the supplier base (Figure 4.3). This internal priority ranking of emission factors should help the company to set up a consistent inventory and consider the company's ambition to reduce their Scope 3.1 emissions and steer their Scope 3.1 target (see 1.2 in Figure 4.4). Guidance for such an emission factor prioritization is provided with the decision tree in Figure 4.5. The selection of certain data sources should consider the availability of data for the internal accounting and target tracking system. Comprehensive information about developing and implementing a Data Management Plan is found in [GHG Protocol Corporate Value Chain (Scope 3) Standard]. A reporting company shall always apply the most specific and accurate available emission factors to ensure the highest quality of the reported Scope 3 Category 1 emissions inventory. To this end, it is recommended to implement a Data Management Plan which can be helpful in the continuous data improvement process but depending on the amount of data it might also help to prioritize efforts (see 1.3 in Figure 4.4). For consistency reasons secondary emission factors should always be taken from the same database, if possible. Furthermore, the reliability of the available data should always be evaluated. An overview is shown in Table 4.3.

Figure 4.4 Key process steps of Scope 3.1 emission factor generation, preparation, and handling

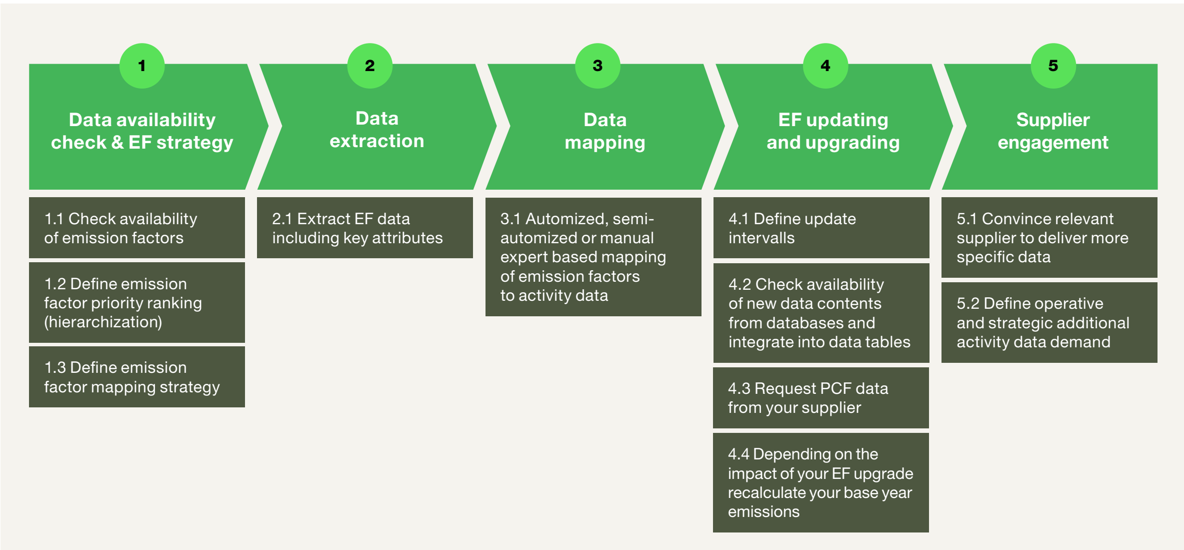


Table 4.3 Overview of data sources available for an accounting of emissions from Scope 3.1

Definition	EEIO	Industry average LCA	Specific PCF	Supplier PCF	Hybrid	OCF*
Description	Sector/country/ global emission factors mapped against purchasing volumes	Product industry average data from LCA databases	Modelled dataset that is more granular for technology or geography than industry average	PCF data per product collected from the specific supplier	Supplier-specific allocated OCF for Scope 1&2 and supplier activity data and average EF data for suppliers' Scope 3	Supplier-specific OCF for Scopes 1, 2, 3 (per EUR or physical units or as abs CO_2 emissions)
Pre-condition	Understanding of corporate spend, currencies, and inflation rates Access to an input/output model	Physical data available Consistent base of LCA data	Detailed knowledge on supply chain incl. physical data PCF data on product level	Willingness of the supplier to share data per product also for baseline	Willingness of the supplier to share inventory data per product (material amounts)	Availability of OCF and purchasing volume data or physical data
Application	Base inventory Hotspot analysis (country, material group contribution)	Broad product portfolio	Capture emission reductions through generic reductions	Measurement of supplier performance Tracking progress to climate goals	General supplier performance	General supplier performance
Source Activity Data	Purchasing records (+ price adjustment)	Reporting company's ERP system BoM	Reporting companies ERP system, BoM	Reporting companies ERP system, BoM	Supplier data	Supplier procurement or ERP system
Source Emission Factors	Environmentally extended Input Output model	LCA database Literature or data on demand	Reporting company or consultancy sector/ product specific model and average LCA data	Supplier PCF based on primary data collection	OCF data for Tier 1 supplier and average LCA/ PCF data for upstream of Tier 1 supplier	Sustainability report CDP report of supplier
Pros	Complete and consistent inventory for all products Good regional coverage	Relatively detailed product differentiation Annual differentiation Easy to access	Detailed product differentiation Annual differentiation	Exact product differentiation	Supplier-specific performance Annual update possible Compromise with respect to effort and data accuracy	Supplier-specific performance Annual update possible Easy and fast to calculate

*OCF = Organizational Carbon Footprint

Definition	EEIO	Industry average LCA	Specific PCF	Supplier PCF	Hybrid	OCF*
Cons	Only coarse product differentiation Time lag of statistical data with the risk of outdated data when used closely before the next update (Inaccuracies due to price and currency effects) No standardization of EEIO models No supplier-specific information	Physical activity data often not complete EF data not available for all products and countries Limited comparability with base year emission due to methodological updates Temporal representative-ness Cost of LCA databases No exact supplier-specific information	Availability of physical activity data Uncertainty in calculation No exact supplier-specific information	Physical activity data often not complete Big effort for data generation, validation and collection, if manually done No annual update, if manually done Limited availability Low traceability if no detailed documentation is available	Large effort for data collection Limited precision Challenging to validate	Inaccuracies and low comparability due to methodological differences (Scope 3) and allocation In case of monetary units sensitive to price and currency effects
Conclusion	Very basic approach. Limitations with regard to accuracy & supplier performance measurement	Basic approach but the more specific the product portfolio the less data are available	Data only available for limited product categories	Highest accuracy with big effort incl. dependency from supplier. However, the effort can be reduced by automating and implementing IT tools for calculating and sharing PCF and PCF data	Medium effort incl. dependency from supplier	Basic approach. Only applicable in case of homogenous product portfolio of the supplier

*** OCF = Organizational Carbon Footprint**

Besides using emission factors of lower data accuracy (e.g., spend or average data method), the reporting company can use sampling and extrapolation methodologies. Using proxy methodologies instead of moving to different data types increases comparability of data within the inventory and thereby improves consistency. Companies should calculate emissions from at least 80% (by volume, weight, or spend – see Table 4.2 for a prioritization approach) of Purchased Goods and Services, after which results should be extrapolated to estimate 100% of emissions. [WBCSD (2013)].

The GHG Protocol identifies extrapolation and proxy techniques as completely legitimate procedures in assessing Scope 3.1 GHG emissions. To estimate the total sum of Scope 3.1 emissions, many companies extrapolate the emissions calculated for a particular part of their purchases to further Purchased Goods and Services with comparable emissions intensity. In the following key approaches for estimation of data are briefly described with their potential application and typical examples. An overview of data sources is shown in Table 4.3.

Table 4.4 Estimation approaches for accounting of emissions from Scope 3.1

Estimation approaches	Application	Examples
Applying more accurate data/calculations for large contributors	If possible, apply a 80:20 approach	Collect primary data from your supplier for 20% of your purchased products that contribute 80% to the reporting companies Scope 3.1 footprint
Applying less accurate data/calculations for small contributors	• Apply industry average PCF dataset of the same product instead of using a supplier-specific PCF • Apply industry average dataset that doesn't have full coverage with respect to technology, geography or time instead of an industry average that has full coverage (proxy)	• Use a "DE: Sodium Hydroxide" dataset from a LCA database to estimate the impacts from your specific sodium hydroxide supplier located in Germany • Use a e.g. GLO or EU average "Sodium Hydroxide" dataset in case of unavailability of a supplier or country-specific industry average
Grouping or combining similar activity data (e.g., Purchased Goods and Services)	Build a group of chemicals based on • SIC or NAICS grouping • Similar chemical structure • Same or similar production technology/process Apply PCF of a product that represents the specific group regarding technology, geography and time	Apply the PCF of methanol to all chemicals that belong to SIC Code 2869 – industrial Organic Chemicals, not Elsewhere classified.
Obtaining data from representative samples and extrapolating the results to the whole	Build a sample making use of simple random, systematic or stratified sampling as described by the GHG Protocol Scope 3 Calculation Guidance, Appendix A	A company purchases 100 products in a specific chemical product category and wants to determine the average PCF, it may choose to collect data from 20 randomly selected products as a representative sample
Using proxy techniques	Extrapolating, scaling up, or customizing to be more representative of the given activity	• A supplier that makes up 80% of the purchased mass of a product can be extrapolated to represent 100 percent of the activity • The emissions of a supplier for sodium hydroxide from Canada is approximated with an emission factor for sodium hydroxide from US

If data of sufficient quality are not available to cover for the minimum 80%, companies may use proxy data to fill data gaps. Proxy data is data from a similar activity that is used as a stand-in for the given activity. Proxy data can be extrapolated, scaled up, or customized to be more representative of the given activity (e.g., partial data for an activity that is extrapolated or scaled up to represent 100 percent of the activity).
[GHG Protocol Corporate Value Chain (Scope 3) Standard]

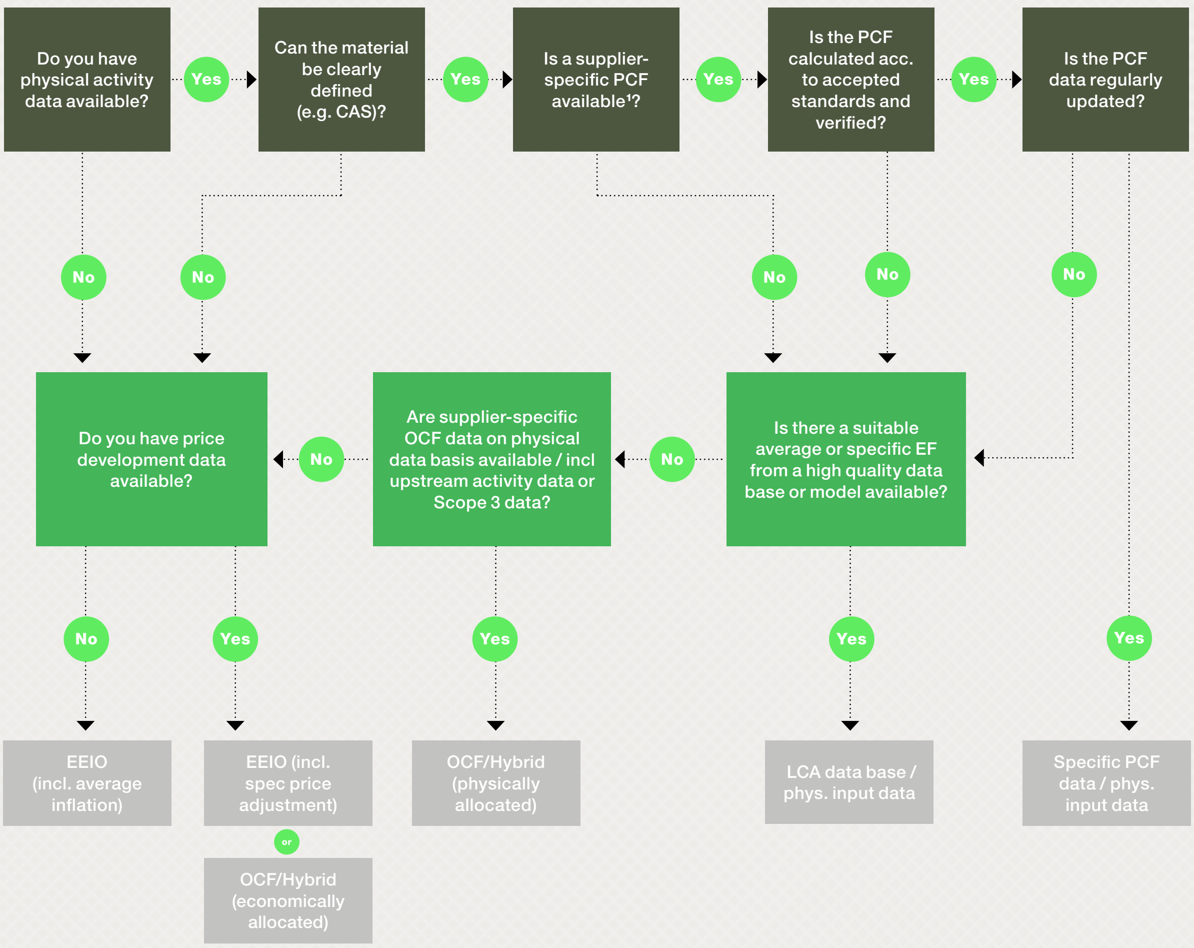
3) Data mapping

Data extraction of emission factors depends on the source the data are taken from. While EEIO data might be taken from public sources or consultancies, PCF data (if not supplier-specific) are usually taken from LCA databases. Since emission factors for the same material may vary by LCA database, a prioritization of databases should be defined that does not allow for the use of too many databases in order to ensure comparability and conistency over the years.

Supplier-specific data are currently most often handed over manually (e.g., excel tables) but will be handed over via predefined tools and interfaces in the future (see the TfS PCF Exchange solution). CDP is also a good source of supplier data, e.g., PCFs and revenue intensity factors. OCF data could be taken from publicly available reports of the suppliers or collected via e.g., CDP or Ecovadis once a year if production amounts and product segmentation is available too. Attributes that describe the emission factors (e.g., geographical, temporal and technological scope) might help to map factors against activity data. Consistent sets of attributes are available with the International Life Cycle Data (ILCD) format available via LCA databases, a format which provides granularity that supplier usually cannot provide, and which is not available for OCF or EEIO data. Attributes relevant for an exchange of PCF data within companies is provided in the TfS PCF data model.

A decision tree supporting the decision process is shown in Figure 4.5.

Figure 4.5 Decision tree to select emission factors (Note: In accordance with chapter 5.2.2 of this guideline, PCFs have a validity period of up to three years and shall be updated before the end of the validity period has been reached.)



(1) Primary and secondary data may be delivered by suppliers. All elements in Chapter 5 need to be considered by the provider of the supplier-specific data. The data should be verified as layed out in Chapter 5.3.

4) Emissions factor updating and upgrading

If manually done, the attribution of emission factors to activity data can be a time-consuming process step. A predefined set of attributes, rules and quality criteria can help to automate (or semi-automate) the mapping process. A final review of a product segment and/or emission factor expert might still be necessary depending on the complexity of the companies purchased material portfolio.

5) Supplier engagement

Reporting intervals require the regular update of emission factors. Due to GHG reduction targets, many companies might strive for yearly updates of their emission inventory (see 4.1 in Figure 4.4). Updates in activity data and emission factors can be actual changes over time, corrections for identified errors, other improvements in data quality, or changes in calculation methodology. Companies shall understand how data are changing and the reason for any changes. It is understood that data quality may be low in initial years of data collection, but companies should strive to improve data quality as quickly and as much as possible in line with their company goals. For the chemical industry, transitioning towards supplier-specific data is one of the most impactful ways to improve data quality. This pursuit could be prioritized for higher use rate inputs and inputs with relatively higher GHG emissions. Suppliers can work intensively on the reduction of the PCF of their products, reducing their own emissions but as well contributing to the reduction of Scope 3.1 emissions of their customers.

Data from LCA databases are subject to a yearly update, while supplier data might be updated less frequently. The requirements on the temporal scope of supplier PCF data are described in Chapter 5.2.2. A process formalization and/or automatization of emission factor update routines can stabilize the process and reduce efforts. The request of PCF data from suppliers might need early planning and exchange with the respective supplier (see 4.3 in Figure 4.4). An emission factor update can also include the upgrade of certain emission factors e.g., the shift from one emission factor source to another. For example, moving from an industry average dataset from an LCA or EEIO database to a supplier-specific dataset in the reporting year could make it necessary (depending on the significance and the company's recalculation policy) to also adjust the base year emissions and any other previous year's calculations with the new emission factor (compare chapter 4.5 on baseline recalculation). To move from using a spend-based method to a more supplier-specific method, a company would need to:

- Eliminate or reduce the spend-based data specific to the purchased good or service of interest from the Scope 3 inventory.
- Use the supplier-specific PCF data if available, or otherwise specific or industry average PCF data instead of this spend-based data in a new Scope 3 calculation.
- Apply this new accounting method to the base year emissions and any previous year calculations.
- This would result in a combination of the calculation methods.

For example, Company A spends a total of $5 million USD each year on Purchased Goods and Services. $100,000 of this spend is for 300 kg of Input Y. While Company A has been using the spend-based method to calculate their Scope 3 emissions, the Supplier for Input Y is now able to provide a PCF for Input Y. The PCF for Input Y is 10 kg CO_2e/kg Input Y. To make this change, Company A follows the below:

$5,000,000-$100,000
= $4,900,000 still using the spend-based method

300 kg of Input Y purchased
x 10 kg CO_2e/kg Input Y purchased
= 3,000 kg CO_2e for Input Y

Total for Scope 3 Category 1 Purchased Goods and Services
= GHG results from spend-based approach for $4,900,000 spend + 3,000 kg CO_2e for Input Y

Companies should encourage their suppliers to develop and report GHG data (see 5.1 in Figure 4.4). A close engagement with the suppliers can help to build a common understanding of emissions-related information and the opportunities and benefits of achieving GHG reductions. An active engagement can assist both parties in better understanding the emission drivers both upstream and during the product's use and disposal. It can also help alleviate concerns regarding the exchange of PCF data. Finally, an operational and strategic demand for emission factors should be defined in the data management plan in alignment with the reporting company's GHG reduction targets (see 5.2 in Figure 4.4).

The Importance of Supplier Data

Decarbonization will not be linear. It will take place at different rates, depending on sector, geography, policy, and market forces. In other words, some companies and products will become low-carbon faster than others. Due to these dynamics, regional and global emissions factors may over or under-estimate the actual emissions of a purchased good. The resulting uncertainty is fast becoming a pressing concern for companies seeking to track progress towards Scope 3 climate goals.

Supplier data is one meaningful solution here, collected via programs like CDP, industry groups, or directly from the supplier. Supplier data can be substituted for emissions factors, multiplied out based on the reporting company's activity data like purchased quantities or spend – for example:

- Supplier PCFs (kg CO_2e per kg of product) for relevant purchased goods
- Revenue carbon intensity factors (kg CO_2e per € or USD revenue) for relevant Purchased Goods and Services

When applying supplier emissions factors, care should be taken to validate that factors were calculated correctly, and are suitable in relation to the methodological background and that they are applied to the correct purchased good or service.

4.5 Scope 3 base year emissions recalculation – Challenges and solutions

Setting clear and achievable climate goals is a crucial step towards sustainable and responsible business practices. Reliable and well-defined base year carbon emissions serve as the foundation for setting meaningful climate goals. It establishes a starting point against which progress can be measured and allows companies to assess the effectiveness of their emission reduction strategies. However, the ever-evolving nature of scientific understanding and data availability necessitates periodic reassessment and adjustment of base year carbon emissions to ensure accurate measurement of progress towards these goals.

This chapter aims to provide comprehensive guidance on when and how a chemical company should recalculate its base year carbon emissions for a corporate climate goal. Aligned with the Greenhouse Gas Protocol, it addresses the scenarios in which base year emissions recalculation and potentially restatement becomes necessary, including acquisitions or divestitures, the reception of new information or data, as well as changes in emissions measurement and reporting methods. By outlining best practices and offering practical recommendations, this document will enable chemical companies to maintain transparency, accountability, and credibility in their pursuit of their climate goals.

Please note that this chapter is relevant to all Scope 3 categories, not only Scope 3.1. The topic of baseline recalculation is overarching and extends beyond a single Scope or Scope category, underscoring its relevance across the entire carbon accounting spectrum.

1) How to start: Establishment of a recalculation policy and determination of base year emissions

Base year emissions are the emissions within the boundary of a climate target in the defined base year. For example, if a company's climate goal is to reduce Scope 3 emissions by 20 % by 2030 versus a 2020 base year, the base year emissions are the company's Scope 3 emissions in the year 2020. Within Scope 3 there can be several targets with their own boundaries and an own defined base year.

According to the GHG Protocol companies shall develop and establish clear internal base year emissions recalculation policies and procedures. This approach creates a consistent benchmark to track emissions reductions over time and to ensure comparability over the years.

A company should establish a base year emissions recalculation policy that defines in detail what triggers a recalculation and what does not. In this context, it is necessary to define what (cumulative) change is considered significant by setting a threshold, where a public restatement of the base year emissions becomes necessary. The GHG Protocol does not specify a particular significance threshold, so the company can establish one for itself, unless it is subject to other requirements in this regard. The SBTi's significance threshold for example is defined as a cumulative change of five percent or larger in an organization's total base year emissions (tCO_2e) (cp. Target Validation Protocol for Near-term Targets, TWG-PRO-002 / Version 3.1, March 2023, pg. 34).

Sometimes recalculation is necessary, but a public restatement is not. A public restatement becomes necessary if the defined significance threshold is exceeded due to a substantial or due to several small changes.

Furthermore, the policy should include a description on how the recalculation shall be performed. Table 4.5 contains an overview of common triggers as well as suggestions for the way of recalculation. It can be used as a starting point and adjusted according to the needs of the individual company.

When base year emissions are recalculated and the emissions are changed significantly as a result, the company shall publicly disclose the updated numbers alongside the reason for the recalculation. In addition, it is crucial to internally document a comprehensive explanation of the reasons, data sources, methodologies, and calculations used to revise the base year emissions.

Recommendation: When a climate target and associated base year emissions are established, the boundaries, scope and the underlying calculations should be as accurate and comprehensive as possible and based on the best available data. Base year emissions recalculations are always time-consuming and can bring a loss of already achieved emission reductions within the supply chain.

2) When to do a Scope 3 base year recalculation

When new information or data becomes available that significantly alters the understanding of carbon emissions within the industry or the company's specific operations, it may be necessary to re-evaluate, recalculate and restate the base year emissions to ensure its alignment with the latest knowledge. For example, scientific research, advancements in emission measurement technologies, and changes in methodologies and regulatory requirements continually expand our understanding of carbon emissions and their environmental impact. Further, if a company undergoes structural changes, such as mergers, acquisitions, divestitures, or the outsourcing of certain business activities, this must also be considered. As a chemical company committed to sustainable practices, it is essential to stay abreast of these developments in the context of one's climate target.

There are several situations that trigger a base year emission recalculation followed by a restatement based on the defined significance threshold. At a high level, there are four common cases that a company may encounter, along with the recommended actions for each:

Mandatory Recalculation: If the company's recalculation policy's significance threshold is reached by a single trigger or by the cumulative effect of multiple triggers over several years, recalculation becomes necessary.

In this case, only the affected categories that caused the recalculation by surpassing the threshold must be recalculated. Categories with insignificant changes can retain their original values. However, to avoid potential future recalculation and restatement due to cumulative changes, it might be advisable to recalculate all categories within the target boundary.

Recommended Recalculation: Recalculation is advised in cases where structural or methodological adjustments result in net emissions changes below the defined threshold but create distortions that limit year-on-year comparability.

Recalculation not recommended: Recalculation is not recommended when cumulative changes in emissions due to one or more triggers cancel each other out, resulting in a net change lower than the significance threshold within the respective Scope 3 category and not affecting the comparability.

Acknowledging Changes: In situations where more accurate data input for past years is unavailable or not applied, such as when using supplier product carbon footprints that do not represent the base year emissions, and the impact of the change itself does not exceed the significance threshold, the change can be acknowledged. The acknowledgment should be transparently documented internally. The company should decide if and how the acknowledgement is disclosed publicly (cp. GHG protocol (pg. 38) regarding further information)

When determining the proper time for recalculation due to cumulative changes, it is suggested to continuously record and track all changes in an internal calculation. This internal tracking calculation should be carried out on an ongoing basis based on the base year emissions and include all methodological and structural changes over time. Comparing the result with the currently stated base year emissions allows then identifying the point in time when the significance threshold is exceeded due to major and minor cumulative changes and thus the moment a restatement becomes necessary.

A first indication to identify significance can also be an estimation of base year emissions using an extrapolation based on spent of the current and base year.

Once the significance threshold is exceeded, the base year emissions shall be officially recalculated and restated, incorporating all changes that led to the deviation, especially in cases of structural or methodological changes.

Example Recalculation & Restatement with cumulative changes:

“Company A has set 2020 emissions as the base year for its Scope 3 target. When it calculates its emissions in 2021, it discovers that there was an error in the activity data in the 2020 calculation, without which the base year emissions would have been 2 % lower. At the same time, to follow current climate science, it wants to switch from the LCIA method IPCC AR5 to IPCC AR6. With this, base year emissions would be 0.5 % higher. However, both changes together do not lead to a significant deviation of the defined base year emissions according to the significance threshold of 5 % defined in the Recalculation Policy of the company. Thus, although the adjustments are taken into account in the calculation of 2021 emissions, the base year emissions are retained. In 2022, the company sells part of its activities. This leads to a reduction in the base year emissions of 4 %. Since the definition of the base year emissions, the base year emissions have thus changed cumulatively by 5.5 %. This is considered material according to the defined threshold and the base year emissions are officially recalculated and restated taking the effect of the 3 structural/methodological changes into account.”

Figure 4.6 Decision tree for identifying triggers for recalculation of base year emissions

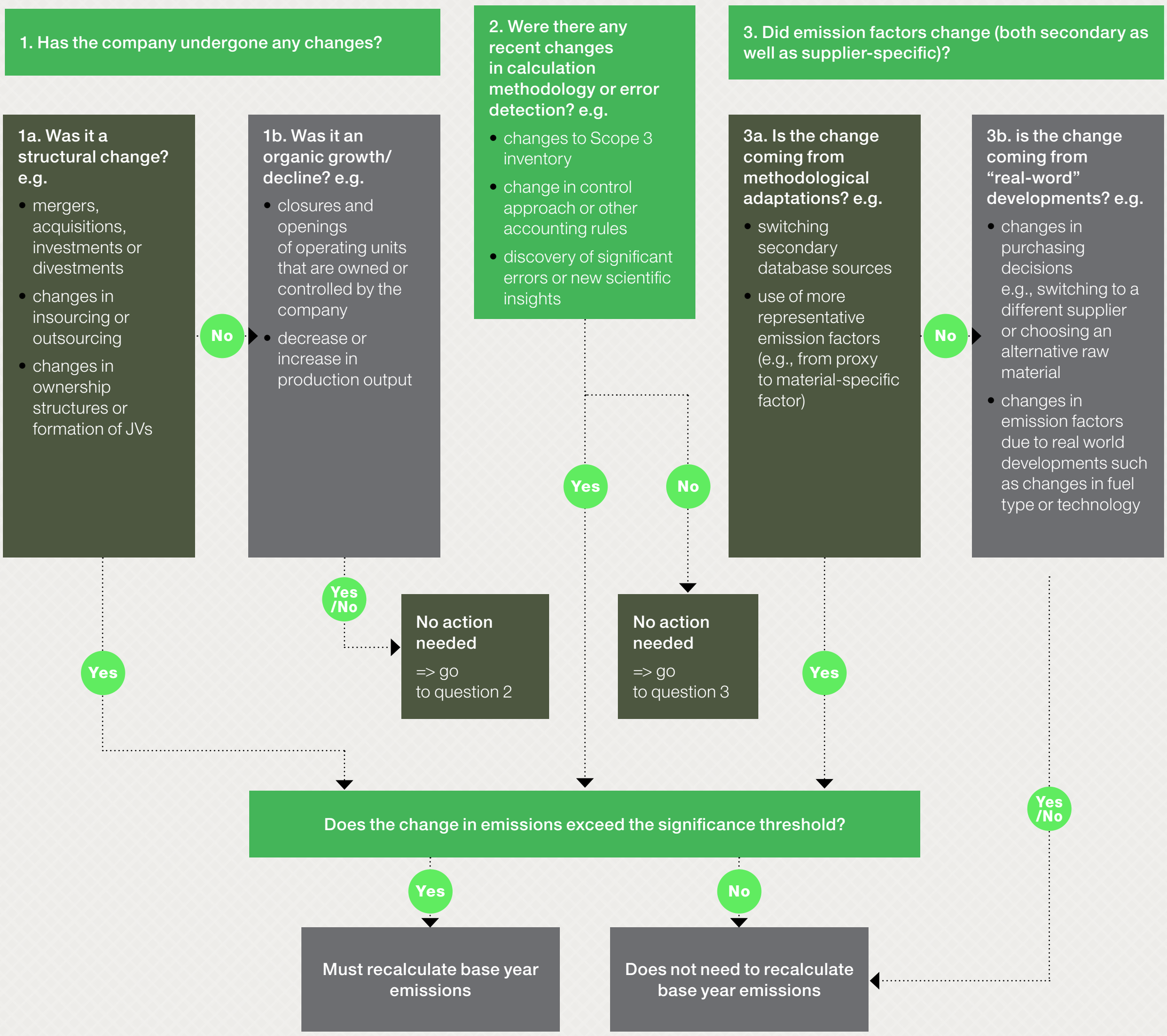


Table 4.5 Overview of activities that trigger a recalculation of base year emissions

Trigger	Definition of Trigger	Comment
Structural[1]: mergers, acquisitions, investments or divestments, changes in ownership of assets/ technologies	Activities which lead to the shift of emissions from one company to another or change the inventory of a company by merging or redistributing emissions due to structural changes or changes to the infrastructure of a company.	Small investments or divestments, such as purchasing individual units or plants previously operated by another company, are unlikely to trigger recalculation due to their low significance. However, it is essential to be mindful of these actions, especially when dealing with more substantial plant components, as cumulative effects may come into play. In case an acquired or divested company, plant, or asset did not exist in the base year, no recalculation of the base year emissions shall be made. If the years between the base year and the year of the acquisition/divestment are recalculated as well, the recalculation can be made up from the year of the existence of the asset. [GHG Protocol (revised), pg. 38].
Structural: Outsourcing/ Insourcing	In- or outsourcing of activities that lead to a shift of emissions from one company to another or between Scopes.	If a company outsources an in-house activity to a third party, the activity shifts from Scope 1 or Scope 2 to Scope 3. Conversely, a company may shift emissions from Scope 3 to Scope 1 or Scope 2 by performing operations in-house that were previously performed by a third party. Whether the outsourcing or insourcing of an activity triggers a base year emissions recalculation depends on whether: • the company previously reported emissions from the activity; • the company has a single base year or GHG target for all Scopes or separate base years and GHG targets for each Scope; and • the outsourced or insourced activity contributes significantly to the company's emissions.
Structural: change in ownership of existing assets/ technologies in case of joint ventures	A part of the business is merged with another company's business into a joint venture.	New establishment and start-up of a joint venture does not lead to recalculation but is considered as organic growth.
Structural: Change to the Scope 3 inventory	Exclude or add a category to the Scope 3 inventory.	If a change is made to the Scope 3 inventory by deciding to include or exclude reporting for a certain category, it is necessary to recalculate the base year emissions. This ensures that the inventory remains comparable. For instance, if a company decides to start reporting on Scope 3 category 10 (Processing of Sold Products), it must include this category in the base year. However, there is an exception to this rule if different base years and targets are defined for individual Scopes and categories. In such cases, the base year and reporting inclusion/exclusion can vary based on those specific definitions [see GHG Scope 3 Standard pg. 101].
Improvement of activity data: Accuracy	Addition of enhanced information for already reported activity data e.g., more detailed information.	**Case 1:** Input of data relevant for emissions calculation is more accurate (e.g., conversion of volume / heating value into mass is standardized) **Case 2:** More detailed/granular activity data is available (e.g., product-specific instead of chemical category data or country-specific instead of regional data etc.) that enables better mapping with respective PCF data (supplier-specific or secondary data).
Improvement of activity data: Completeness	If any new information becomes available or is learned, additional activity data should be included.	**Example:** A company closes data gaps due to an enhancement of their Enterprise Resource Planning (ERP) system. Hence, activity data is more complete.

(1) GHG Protocol revised: "Structural changes in the reporting organization that have a significant impact on the company's base year emissions. A structural change involves the transfer of ownership or control of emissions-generating activities or operations from one company to another. While a single structural change might not have a significant impact on the base year emissions, the cumulative effect of a number of minor structural changes can result in a significant impact"

How to recalculate (recommendation)

- Include or exclude the emissions of the activity
- If it is not possible to make a recalculation in the year of the structural change (e.g., due to lack of data for an acquired company), the recalculation may be carried out in the following year. [GHG Protocol revised, pg. 37f.]
- If the emissions of a newly acquired activity remain unknown in the following year due to lack of detailed activity data of the base year, an estimate for the base year emissions shall be done based on the best available data to account for aquired companies or plants that did not exist in the base year.

Example acquisition of (parts of) another company: In case no emission data is available, one option is to use the revenue of the former years multiplied by the acquired company's ratio of emissions per revenue (tCO_2e/€).

Alternatively, the emissions for the base year can be calculated based on the initially available actual activity data after the structural change, adjusted by the ratio of the revenue of the actual year compared to the base year.

Example: An asset of a purchased company did not exist in the base year of the investing company:

Company A purchased a portion of Company B in 2022, comprising five plants. However, during Company A's base year in 2019, one of the plants (Plant 5) did not exist; it was built in 2021. In the recalculation of Company A's base year emissions, Plant 5's emissions will not be taken into account. Instead, the emissions from Plant 5 starting in 2021 will be treated as organic growth and have to be accounted for in the regular GHG emissions inventory of the company.

If emissions shift to categories that have not been previously reported, an estimate must be made. This estimate can be based on internal information or information provided by a service provider.

Note that a new or revised tolling agreement could lead to a significant shift in emissions between Scopes. In cases where there is no overarching climate target across the affected Scopes, a recalculation may be necessary. In case there is an overarching climate target across multiple Scopes in place, no recalculation is necessary.

In case existing parts of two or more companies are merged into a joint venture, the emissions must be calculated according to the operational or financial control of the joint venture. If operational or financial control no longer applies to the former fully owned activities of the newly founded JV, a shift in Scopes occur towards 3.15 and recalculation might be needed if the significance threshold is exceeded.

Case 1 The company decides to no longer report a certain Scope 3 category: The category is excluded at least for the current reporting year as well as from the base year.

Case 2 The company decides to report a new Scope 3 category: The category shall be calculated at least for the current reporting year as well as for the base year. If the activity data required for the recalculation of the base year are missing, a suitable approximation should be chosen.

Example category 10: To estimate the emissions for this category in the base year, one can extrapolate the emissions using the sales data from both the current reporting year and the base year.

If the share of the newly calculated category is an insignificant share of the inventory (according to the reporting company's defined approach to significance thresholds) and a suitable approximation of the base year emissions cannot be found, one approach may be to use the current reporting year to represent the base year.

Assess the applicability of new activity data for the base year to understand if the data fits the time period of the base year and if a similar resolution can be defined (e.g., if new data is based on region, assess the availability of regional data in the base year). If determined applicable, apply the new and improved conversion factors for activity data of the base year to recalculate the base year emissions.

If the data is not available in a similar resolution, check whether it is possible to draw conclusions from existing data to the data in the base year and apply if appropriate and reasonable (significance criterion).

- Verify if any data still needs to be collected in the base year or if additional data from other sources is required. If data is missing or needs supplementation, use newly acquired or collected data to complete the base year emissions calculation.

- If it is no longer possible to collect data for the base year, but recalculation is still necessary due to significance and relevance, transfer data from the current year to the base year. If feasible, rescale the data, for example, by comparing the amounts of applicable activity data between the current year and the base year.

Trigger	Definition of Trigger	Comment
Methodological changes: Change in control approach (financial / operational)	If a company's organization boundaries or control approach are changed.	The GHG Protocol describes three distinct options for defining a company's organizational boundaries, which in turn impact how GHG emissions are consolidated. For example, a company that previously used the equity share approach might decide to switch to an operational control approach due to legislative requirements. This change means that the company must now account for 100 % of the GHG emissions over which it has operational control, and this will consequently affect the overall calculation of Scope 1-3 GHG emissions.
Methodological changes / improvements – calculation method	There are several ways to calculate the emissions of a category, depending on the used database or with respect to the extrapolation approach to estimate a part of the emissions for which appropriate data is not available. If the available information needed for calculation improves a change of the calculation method can be useful to reach a higher level of accuracy.	Methodological changes such as the following can trigger a base year emissions recalculation: **Case 1:** A company changes its calculation method from a spend-based method (emissions are estimated based on the economic value of a product and a revenue-based emissions factor) to a more accurate average data method (emissions are estimated based on quantity a weight-based emissions factor) or supplier-specific method (applying PCF data from suppliers). **Case 2:** Change in extrapolation step. **Case 3:** Change in reporting rules; new guideline.
Methodological changes/ improvements - database change or use of improved emissions factors	An exchange of one or more emission factors based on more current or precise data, without necessarily correlating with an actual improvement or deterioration of the climate impact of a product or service.	**Database Change:** Change from one emissions database to another **Case 1:** A company replaces a dataset from a secondary database to supplier-specific data. **Case 2:** A company changes a database source, e.g., because the PCF value from the new database is a better match, i.e., is more appropriate and better reflects the technology used or production geography for the raw material purchased. **Improvement** An improvement is an exchange of a PFC by another PCF with a better quality, e.g., that is more complete or better reflects the actual production situation or production geography.
Methodological changes/ improvements – Change of LCIA method	A change of the LCIA method can occur if a company previously reported emissions using a certain LCIA method decides to switch to another method e.g., to ensure actuality with the latest IPCC report.	**Example:** Change from CML2001 – 2016 (using characterization factors according to IPCC AR5) to a LCIA method which contains the latest characterization factors according to IPCC AR6.
Methodological change: allocation approach (emission factors)	Allocation approaches (the partitioning of emissions and removals from a common process between the studied product's life cycle and the life cycle of the co-product) may change due to regulatory requirements or voluntary standards/guidelines. Hence the resulting emission factors undergo a change.	**Example:** An LCA databases adopts the allocation principles of the TfS PCF Guideline. Individual CO_2e factors per kg of product are affected and significantly differ from the previous values.
Discovery of significant errors	Errors can be internal or external.	**Example 1:** A company uses performance data that has been entered incorrectly in the ERP system, e.g., due to an error in unit conversion. **Example 2:** A company uses supplier-specific PCF values that contain a calculation error.
Change in emission factors: New scientific insights	Change in emission factors caused by commonly acknowledged new scientific insights or studies, but also due to a change from one LCIA method to another.	**Examples:** • Change of characterization factors due to new IPCC reports, • Emissions from natural gas and oil extraction are higher than assumed until 2019, affecting the majority of the fossil based raw materials' emission factors in commonly used databases.
Change in accounting rules	Accounting standards like the GHG protocol are adjusted from time to time to reflect new scientific findings and to correct or specify existing content. This may require an adjustment of previous calculation methods.	**Example:** The release of the GHG Protocol Land Sector and Removals Guidance could change the way that biogenic CO_2 emissions are considered.

How to recalculate (recommendation)	
Recalculate by applying the new organizational boundaries and consolidation approach.	
Recalculate base year emissions according to new approach. PCF data that is needed for the recalculation of the base year emissions should ideally reflect the situation at the time of the base year (please see below “methodological improvements – database changes” for further guidance how to obtain corresponding PCF data).	
The recalculation requires PCF data that was valid at the time of the base year. This refers to information from PCF databases as well as supplier-specific data and improved emission factors. 1) Ask database provider or supplier for PCF data from base year 2) If not available, ask supplier if significant changes have occured 3) No changes or if no information is available: use data from current year (= year the PCF was obtained for the first time) data also for base year (loss of efficiency gains possible) When considering diverse and granular inventories, especially related to Scope 3 Category 1, recalculation triggered by a shift from secondary to primary data may become undue effort.	Reasons for this are: • **Primary data** related to the base year is not easily available, • **Secondary data** may be a better approximation of the base year emissions than the current supplier-specific data since it could be less representative than the secondary base year data. For such cases, a company can decide on a threshold under which the methodological change for an activity will not trigger recalculation. Such threshold should be disclosed together with the aspects listed in section 3. (disclosure section – internal as part of a company’s recalculation policy). To determine if the threshold is exceeded, the difference in the GHG impact of the supplier-specific and secondary data in the current year needs to be calculated. In case the threshold is exceeded, further investigations into additional information on the three options listed above is required.
The emissions of the base year should be calculated with the emission factors of the previous and the future LCIA method. If the impact is significant according to the significance threshold as defined in the recalculation policy, a recalculation or a or restatement of base year emissions shall be carried out.	
To ensure accuracy, significant changes that impact a company’s emissions require PCF data calculated based on the current allocation approach for the base year. This also applies to supplier-specific PCF information. However, if the updated PCF data is not available for the base year, the PCF data from the current year (= year the PCF was obtained for the first time) can be used for the base year emissions.	For companies dealing with a large portfolio of different raw materials, this process can be challenging. In such cases, it may be more practical to focus on the raw materials that contribute the most to the Scope 3 emissions, following the 80:20 rule (focusing on the raw materials making up 80% of emissions).
If significant, a recalculation is required, which eliminates the error. New and corrected supplier data are to be updated.	
In order to assess the impact of the updated emission factors, it is necessary to estimate the effect on emissions by utilising activity data from base year in conjunction with the revised emission factors.	If significant, a recalculation of the base year emissions is required using the activity data of the base year in combination with the updated emission factors.
The calculation must be performed following the new accounting rules after release of the revised or additional guiding standard or after a certain officially determined transition phase. If the change in accounting rules leads to such a difference in emissions so that comparison is no longer possible (e.g., due to different reporting requirements) or the significance threshold is reached, a recalculation of the base year emissions is necessary.	• **Example 1 - More detailed information required:** The additional information shall also be calculated for the base year to ensure comparability between the reporting year and base year. • **Example 2 - Change in approach for calculating a certain category:** The emissions for the current reporting year can be calculated using both the old and new calculation approaches. If the difference in calculation does not significantly impact the results, a recalculation is not required.

Table 4.6 Overview of activities that do not trigger a recalculation of base year emissions

No recalculation is triggered by…	Reasoning
Organic growth or decline.	Base year emissions and any historic data shall not be recalculated due to organic growth or decline. Organic growth or decline refers to increases or decreases in production output, changes in product mix, and closures and openings of operating units that are owned or controlled by the company. The rationale for this is that organic growth or decline results in changes to the company's emissions profile over time, which must be accounted for as increases or decreases in emissions to the atmosphere [GHG Protocol Corporate Standard, revised].
Change in generic or supplier-specific emissions data (PCF) over time.	According to the GHG Protocol Scope 3 Standard, page 106, recalculations are not necessary for changes in emission factors that result from real changes in emissions or activities, such as changes in fuel type or technology.
Change in the purchasing decision e.g., purchase of the same raw material produced with a different technology or in a different region or based on a different feedstock. The new emission factor can be still from a secondary database or supplier-specific.	See also above. The decrease of a CO_2e emission factor or PCF value, respectively, that is based on a real improvement, e.g., through implementation of energy efficiency measures, use of renewable electricity, or change in technology or geography does not trigger a recalculation. These improvements are considered real reduction measures that can be counted towards a set reduction target. The same is true for the opposite effect, i.e. an increase of the emission factor due to deterioration in efficiency, change in production technology or other circumstances.
A change of supplier or the provision of an updated PCF of the same supplier for the same raw material does not lead to a recalculation if the PCF of the new replaces the PCF of the former supplier-specific PCF (in contrary to the exchange of a database PCF by a supplier-specific PCF without any real improvements).	Same as above. Any changes in emission factors or activity data that reflect real changes in emissions (i.e., changes in fuel type or technology) do not trigger a recalculation.
Structural changes in the reporting company's activities resulting in the transfer of emissions between scopes or categories, provided that all affected scopes and categories are reported by the company, share the same base year, and have the same target ambition.	The GHG protocol describes the case of 'outsourcing/insourcing' as structural change that can lead to a transfer of emissions between different scopes. According to the respective paragraph, it is assumed that a recalculation is not necessary if "the company is reporting its [indirect] emissions from relevant outsourced or insourced activities", and as far as no significant emissions are shifted between different scopes in case the emissions of all affected scopes are tracked together over time and refer to the same base year (cp. GHG protocol revised, pg. 38). There might be further kind of structural changes which could lead to a transfer of emissions between scopes or categories on which the same approach could be applied. However, if scopes are tracked or reported separately, refer to different base years and/or underly different target ambitions, a recalculation is necessary.

3) What to document internally

To make decisions for or against a base year emissions recalculation, possibly followed by a restatement, potentially spanning multiple years, it is important to document and justify significant one-time decisions, and potentially support them with calculations. For recurring smaller decisions, such as the use of supplier-specific PCFs in different contexts, it may be useful to establish rules, write them into the base year emissions recalculation policy, and consistently follow them. In this case, only exceptions to the general rules would need to be separately documented, for example as comments in a database or changelog. An internal calculation as mentioned above is recommended to keep track of several small changes and their cumulative effect over time. The recalculation policy should also define a timeline for recalculation after a trigger occurs. The recalculations should be aimed as soon as possible with a reasonable effort. The GHG Protocol Scope 3 Standard allows for a recalculation in the year following a structural change. In alignment with this standard, recalculation can be carried out for the full reporting year after a structural change and therefore a trigger occurred. This will help to allow for time to collect data for a full reporting year and possibly eliminate assumptions on historic data.

4) What to disclose in external reporting in terms of base year emissions recalculation

When reporting publicly base year emissions, the related targets and the current GHG inventory the following information shall be given at a minimum in case of recalculation:

- Information that a recalculation took place
- General reason for the recalculation (structural change, methodological change, activity or emissions data improvement, correction of errors, …)

In case of structural changes, a link can be given to information that is already publicly available, e.g. "due to divestment of company part XY". Significant methodological changes may be disclosed, for instance a database switch.

5) Conclusion & Summary of advises given

In the pursuit of corporate climate goals, chemical companies must recognize the importance of periodically re-evaluating and restating their base year carbon emissions. By doing so, companies can accurately track progress, adapt to new information and methodologies, and demonstrate a commitment to sustainability and environmental stewardship. By following this practical guidance and best practices, chemical companies can navigate the complexities of adjusting their base year carbon emissions, ensuring credibility and transparency in their journey towards a more sustainable future.

4.6 Additional accounting and reporting guidance

In the chemical industry specific cases must be dealt with as they are not covered by the accounting approaches of accounting. In this sense, the following topics are covered, and the procedures described. The challenges of avoiding double-counting as much as possible, the accurate data handling and the accounting in specific situations are described.

4.6.1 Contract manufacturing including tolling

Principles of emissions reporting for contract manufacturing activities:

- Outsourcing of production steps shall not lead to outsourcing of product-related emissions while ensuring that double-counting is minimized at the same time.
- The information needed to calculate emissions should be obtainable with a reasonable effort (in the worst case e.g. applying spend-based approach under consideration of chapter 5.2.11.2 for data quality).

Description of terms:
A **contract manufacturer** is a manufacturing company of a product on behalf of another company (client) for which it produces the contract manufactured goods using its own assets. The raw materials, energies, utilities needed to produce the contract manufactured product are either completely purchased by the contract manufacturer or partially purchased, or fully provided by the client.

A **toll manufacturer** is a contract manufacturer as defined above but who produces on behalf and under consideration of the intellectual property of another company (client).

The **client** is the company that has outsourced the production to the contract manufacturer.

4.6.1.1 Contract manufacturing with raw materials, energy and utilities etc. procured exclusively by the contract manufacturer

From a GHG accounting perspective, contract manufactured products (CMP) for which raw materials, energies and utilities are exclusively purchased by the contract manufacturer shall be treated like trading goods or any other purchased raw materials:

$$Emissions_{Scope3.1} = Mass_{CMP} * PCF_{CMP}$$

The contract manufacturer should calculate the PCF of the manufactured product (see Chapter 5 for guidance to calculate PCF) and provide the PCF to the client, the reporting company, but in case no manufacturer-specific PCF is available a database PCF value or proxy can be used (please see 5.2.5: data types & sources).

4.6.1.2 Contract manufacturing with raw materials, energy and utilities etc. partially purchased by the contract manufacturer or fully provided by the client

In contract manufacturing, in which raw materials, energy and utilities are only partially purchased by the contract manufacturer or fully provided by the client, the calculation of Scope 3.1 emissions differs depending on the level of detail of emissions data provided by the contract manufacturing company as well as on the extent of raw materials and/or energy provided by the client to the processes of the contract manufacturer.

The emissions and resulting PCF should be calculated based on activity data, collected by the contract manufacturer using primary or secondary emissions data and on information about the emissions of the raw materials and energy provided by the client. Generally, activity data should not be requested by the client if there might be any antitrust implications.

Concerning raw materials, energies etc. provided by the client – the assumption and precondition for the following suggested calculation rules are that the emissions for these raw materials and energies are already considered in the greenhouse gas inventory of the client, e.g., in Scope 3.1 or Scope 1 or 2 emissions.

Based on the exchange of aggregated PCFs, no extraction of activity data is possible. However, in case PCF values of precursors are sent by the client to the Contract Manufacturer, GHG emissions associated with the manufacturing process, e.g. from energy use, shall be added to the PCF by the Contract Manufacturer in a new PCF calculation. The Contract Manufacturer should then provide a new PCF to the client to reflect the manufacturing process. It should be avoided, that business critical information can be extracted from the calculation. This guideline is not meant to violate any applicable law or antitrust thus we recommend every company when exchanging partial PCFs to check with their legal advisor on compliance.

Double-counting of emissions from the contract manufactured product ordered and received by the client and from the raw materials purchased and provided by the client should be avoided but is generally acceptable. However, if more precise information is available, this shall be used to reduce the degree of double-counting.

Depending on the provided information the following approaches shall be applied, whereby the provision of primary data regarding the contract manufactured product is always to be preferred:

1) If a PCF calculated by the contract manufacturer for the contract manufactured product based on activity data and primary or secondary emissions data cannot be provided by the contract manufacturer, a carbon footprint of a database, a proxy or an estimated PCF shall be used to calculate the emissions from contract manufacturing. This generic PCF shall not be adjusted according to the client's known volume of energy and/or materials provided by the client to produce the product to avoid mistakes / missleading modeling due to unknown assumptions of the generic PCF.

2) If the contract manufacturer can provide a full cradle-to-gate PCF, the reporting company (client) shall calculate the emissions according to one of the following options:

   2a) The emissions of the contract manufactured product are calculated using the cradle-to-gate PCF provided by the contract manufacturer whereby the emissions caused by energy and/or raw materials provided by the client are subtracted from the respective Scope 3.1 emissions by the client reporting the emissions. In case raw materials produced by the client are provided to the contract manufacturer, the PCF of the contract manufactured product can be reduced by the emissions per kg of the provided products considering the share of the raw material produced and provided by the client necessary to produce the contract manufactured product.

   2b) The Scope 3.1 emissions linked to contract manufacturing are calculated using the cradle-to-gate PCF provided by the contract manufacturer whereby the emissions caused by energy and/or raw materials provided by the client are double-counted.

3) If possible, the contract manufacturer should provide a cradle-to-gate PCF already reduced by the energy/materials provided by the client helping to avoid double-counting. In this case, the emissions caused by energy and/or raw materials provided by the client must not be subtracted by the client when calculating and reporting the emissions.

In case that

1) At least a share of 90% of the mass of the raw materials (always including catalysts and other high GHG-intense raw materials), energies and utilities are provided by the client.

2) And it is assured that the contract manufacturer does not deploy any GHG-intense raw materials, e.g. catalysts.

The following additional option to calculate the emissions can be followed:

The contract manufacturer should provide the client with information on direct emissions as well as emissions caused by waste and wastewater treatment in [kgCO_2e/kg] during the production of the contract manufactured product. In this case the client shall only take these additional emissions mentioned in the sentence before into account within Cat. 3.1.

If the contract manufacturing process is well known, the client itself should calculate the direct emissions as well as the emissions caused by waste and wastewater treatment based on fuel consumption and stoichiometry and subtract the emissions from the Cat. 3.1. emissions.

Special Case "Outsourcing of 1 Minor Process Step":

One minor production step is outsourced to another company (contract manufacturer) e.g., simple mechanical, thermal processes, or chemical reactions. The raw material or intermediate product is delivered to the contract manufacturer for processing and purchased or taken back by the client after the conversion. Transport emissions and possible packaging etc. need to be included. Both raw material or intermediate product and processed product are recorded in the internal booking system (e.g. ERP system).

The following accounting methods can be applied:

1) The emissions are calculated using the cradle-to-gate PCF of the contract manufactured good after the outsourced process step. The emissions or the purchased volumes of the raw material / intermediate product which was the initial material are subtracted from the Scope 3.1 emissions.

2) The emissions are calculated using the PCF of the raw material / intermediate product as well as the partial PCF of the outsourced process step. If the partial PCF of the outsourced process is not known it shall be estimated for the essential (e.g., by spend, by mass or by energy intensity) process steps to be identified via a hotspot analysis (80:20 approach). The thus determined, mass/spend/energy weighted PCF should be used to estimate the not yet considered emissions from nonessential process steps. If the product is additionally tracked in the ERP system after the processing step, its emissions should be subtracted from the Scope 3.1 emissions to avoid double-counting because listed in different systems.

3) If (partial) PCFs that cover only parts of the whole life cycle, e.g. cradle-to-gate. as defined in ISO 14067 are not available for products from the outsourced process and/or the raw materials before the outsourced step, double-counting is accepted and should be disclosed as such. The purchased as well as the processed material shall be considered in the final extrapolation step to account for 100% of the sourced materials (see chapter 4.4).

In case the contract manufacturer is the reporting company, all emissions which are caused by the production including the emissions for the upstream (as Scope 1, Scope 2 and Scope 3.1 emissions, respectively) shall be reported including the raw materials/energies etc. that were not purchased but provided by the client free of charge.

4.6.2 Trading of materials/Merchandise

In case a chemical company conducts trading activities in addition to its core business, it shall report the related emissions under Scope 3, notably categories 1 (Purchased Goods and Services), 4 and 9 (Upstream and Downstream Transportation and Distribution), 11 (Use of sold products – if applicable) and category 12 (end-of-life treatment of sold products).

If, however, the trading activity does fulfill the definition of a spot transaction, thus a chemical company is taking and making physical delivery within (a) a symbolic second as a participant in a back-to-back transaction chain (b) two trading days or (c) the period generally accepted in the respective product market as the standard cargo delivery period, the chemical company may exclude the respective GHG emissions from its Scope 3 inventory. For the avoidance of doubt, relevant for the time determination is the elapsed period between the transfer of title of the buy transaction and the transfer of title of the respective sell transaction.

The facts and circumstances of transactions eligible for exclusion should provide reasonable evidence that:

- The final purpose of the respective purchase and sell transaction is not the interest in the ownership of the physical product for e.g. physical distribution, physical storage, physical blending and/or physical consumption any longer.
- The frequent change of the very short term “interim ownership” of the material and the consequential subsequent reporting by each interim product owner would trigger a high level of double-counting of the same CO_2 emissions in multiple Scope 3 calculations. Inevitably leading to a systematic inflation and incorrect CO_2 emission data reporting across multiple industries.

4.6.3 Swaps

Swaps* are goods transactions, in which products are mutually delivered or exchanged, respectively, between two business partners (third parties). Usually, identical, or equivalent products are swapped in equal quantities. These mutual delivery transactions are generally carried out as they are beneficial for the swap partners, e.g., due to:

- Optimization of logistics (e.g., savings in freight, tank, and customs costs) or
- Compensation for temporary product bottlenecks or surpluses.

In the case of a swap agreement, the reporting company shall report the scope 1 and 2 emissions of its own operations, related to the manufacturing of the product in question:

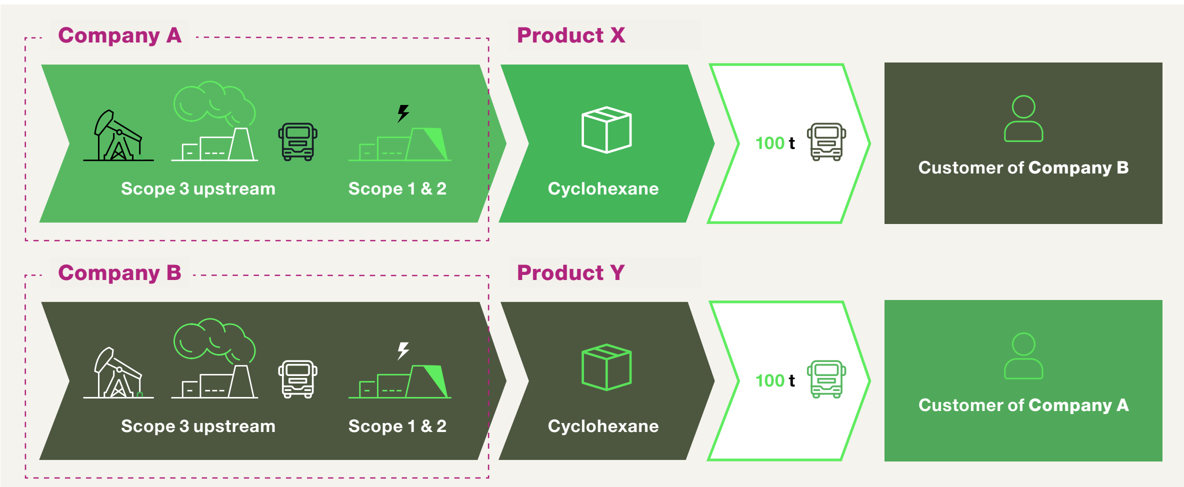
- The scope 1 and 2 emissions from the swapping partner shall not be reported in the scope 1, 2 or 3 inventory.
- Chemical companies may separately report the emissions of the partner company in case of swap arrangements.

An example for a swapping agreement related to a chemical product is given as follows. Company A located in Europe produces Product X and Company B located in Asia produces Product Y. Both companies enter into a swapping agreement and Company B sells Product X (manufactured by Company A) to their customers in Europe and Company A sells Product Y (manufactured by company B) to their customers in Asia.

Different cases of swapping agreements are to be distinguished, i.e., whether equal and comparable quantities, respectively, or different quantities of a chemical product are exchanged over the period of one year (i.e. in the annual balance sheet).

For all swap arrangements, each of the companies shall account for their own Scope 1, 2 and 3 emissions linked to their product, i.e., Company A accounts for and reports the Scope 1, 2, and 3 upstream emissions related to the production of Product X and, respectively, Company B to produce Product Y. This means that both companies involved in the swapping agreement consider in Category 3.1. the GHG emissions linked to their own raw material purchase, and not the raw material purchase related to the product that is physically delivered to the customer because of the swapping agreement. Only the GHG emissions from transportation from the swapping partner to the customer shall be reported by the selling company (in Scope 3).
All swaps should have similar properties. i.e. swap fossil with fossil-based products and bio with bio-based products. Only materials are swapped and the PCFs are calculated separately as shown in the example. Example 2 is shown in Figure 4.6. Swapping does not affect the PCF calculation for either the receiving or sending company.

Figure 4.6 Same product with about the same quantities are swapped, example 1



*according to source: [Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain, WBCSD 2013; ISBN no 978-2-940521-03-6].

Company A accounts and reports:

1. The Scope 1, Scope 2 and upstream Scope 3 emissions related to the production of the 100 tons of cyclohexane (Product X).

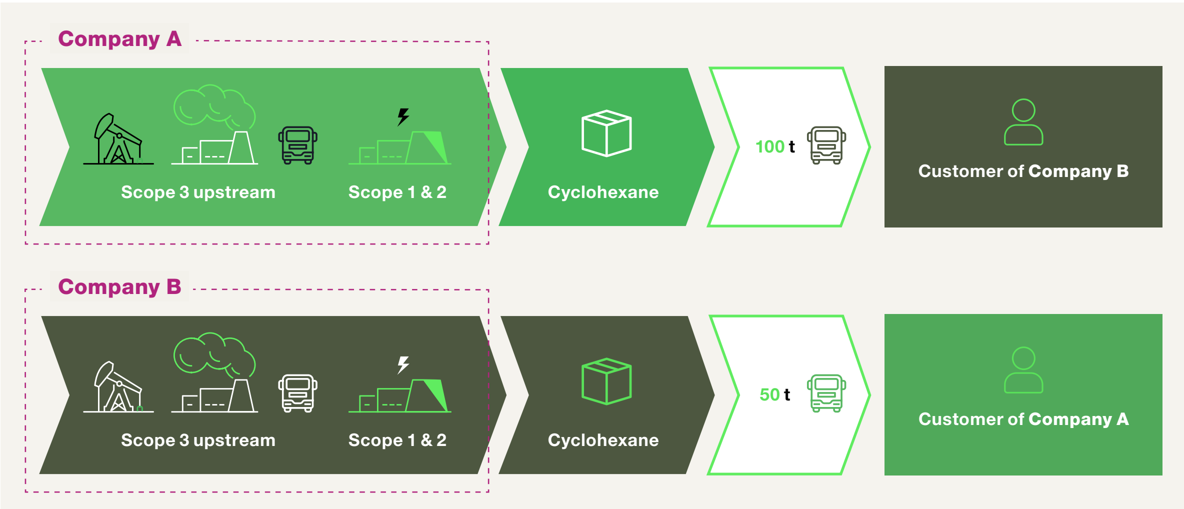
2. The Scope 3 emissions related to the transport of 100 tons of cyclohexane (Product Y) from the swapping partner (Company B) to its customer.

For company B it is the same vice versa.

The PCF communicated to the customer is the PCF for the same product of the selling company. This means that e.g., the customer of company B receives the PCF of the cyclohexane produced by company B and not the PCF for the delivered product from Company A.

This ensures that a company communicates to its customers only a PCF, whose calculation, and data basis it is responsible for. In addition, customer communication remains consistent, even when the swapping partner changes. It also offers no incentive to swap products with high carbon footprint. Example 1 is shown in Figure 4.6.

Figure 4.7 Different quantities of the same product are swapped, example 2



Company A accounts and reports:

1. The Scope 1, Scope 2 and upstream Scope 3 emissions related to the production of the 100 tons of cyclohexane (Product X).

2. The Scope 3 emissions related to the transport of 50 tons of cyclohexane (Product Y) from the swapping partner (Company B) to its customer.

Company B accounts and reports:

1. The Scope 1, Scope 2 and upstream Scope 3 emissions related to the production of the 50 tons of cyclohexane (Product Y).

2. The Scope 3 emissions related to the transport of 100 tons of cyclohexane (Product X) from the swapping partner (Company A) to its customer.

3. The cradle-to-gate GHG emissions linked to the differing amount of 50 tons from Company A as purchased raw material in category 3.1.

To compensate for the difference in the quantities in the respective company balance sheets, Company B, which has produced only 50 t in real terms but has sold 100 tons of cyclohexane to its customer, must account for the cradle to-gate GHG emissions linked to the "missing" 50 tons as purchased raw material in category 3.1*.

The PCF communication to the customer follows the same rules as in case 1.

*There is a difference in PCF and Scope 3.1 accounting.

4.6.4 Joint ventures/Joint arrangements

This section intends to clarify how to account for GHG emissions for products made from joint operations, joint ventures, or other structures where there is a joint responsibility between two or more companies. It describes how impacts of production processes for this type of company relationship shall be considered for Purchased Goods and Services.

The approach to be taken differs depending on the accounting approach chosen by the company in line with the approaches specified in the Greenhouse Gas Protocol Corporate Standard. Companies are encouraged to align their GHG accounting with their financial reporting as recommended by the Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain (WBCSD, 2013). This approach ensures internal consistency of GHG information with reported revenue (Table 4.5).

4.6.5 Recycling/ recycled content (what to report where: category 3.1 vs. category 3.12)

A waste is any residue of a production operation, transformation or use, any substance, material or object, which the holder discards or intends or is required to discard. The term secondary material is used for types of waste that can be used, recycled, reused again before final disposal. The efforts needed and the subsequent GHG emissions to recycle those materials can be linked to the input and the generated secondary materials in different ways. Chapter 5.2.8.4 gives guidance on how PCF data for recycled materials should be calculated. If companies buy and use materials derived from recycling, the share of the recycled content shall be reported including the PCF.

The emissions of recycling or recycling contents can be accounted in different categories:

A) If a company purchases a product or material that contains recycled content (up to 100%), the upstream emissions of the recycling processes are built into the cradle-to-gate emission factor for that product and would therefore be reflected in category 1 (Purchased Goods and Services). If a company purchases a recycled material that has lower upstream emissions than the equivalent virgin material, then this would register as lower emissions in category 1. Under circumstance described in bullet B), a company may recycle some of its “operational waste”.

B) On the other hand, products with recyclable content eventually become waste, which could be recycled. Emissions generated in this process are reported as category 12 (end-of-life treatment of sold products).

To allocate the emissions to different companies and categories correctly and consistently, and to avoid double-counting, a standardized method which sets consistent boundaries is needed.

Adhering to the hierarchy of waste for Scope 3 accounting and reporting, **the recycled content method** (described in detail on p. 77 -79 in the *Technical Guidance for Calculating S3 Emissions* provided by the *Greenhouse Gas Protocol Protocol [WBCSD (2013)]*) shall also be applied by companies. According to this method, recycling processes shall be included in Cat. 3.1 (Purchased Goods and Services) of the company purchasing and using the recycled product.

The implications for category 3.12 (end-of-life treatment of sold products) are the following:

- Companies shall only account for emissions from the first lifecycle of the product, not for any emissions following the recycling of the product.
- The emission factor for recycled products and the allocated share of energy recovery will be reported as zero.

The recycled content method is generally consistent with secondary emission factors available for recycled material inputs and therefore easy to apply.

Table 4.7 Overview of equity share and control approaches

Equity share approach		Equity share included as part of company’s Scope 1 and Scope 2 GHG accounting
Control approach	Operational control approach	Included in company’s Scope 1 and 2 GHG accounting if joint venture is under company’s operational control, OR Included in company’s Scope 3 (category 15) if joint venture is not under company’s operational control
	Financial control approach	Equity share included as part of company’s Scope 1 + 2 GHG accounting if joint venture is under company’s financial control, OR Included in company’s Scope 3 (category 15) if joint venture is not under company’s financial control

4.6.6 Biogenic emissions and removals

The guiding principles for establishing biomass and mass balance products in the accounting for the chemical industry are described in Chapter 5.2.10.5. In addition, the Chapters 5.2.10.1 until 5.2.10.2 and 5.2.10.5 provides further guideline for calculating the PCF for biogenic removals and carbon.

4.6.6.1 Biogenic Emissions and Removals in Cradle-to-Grave Product LCAs

According to the European Commission Product Environmental Footprint (PEF 2021) system and the [GHG Protocol Product Standard], biogenic CO_2 emissions and biogenic CO_2 removals are considered as neutral, independently from end-of-life treatment. The CO_2 removal is balanced with the CO_2 emissions at the end-of-life (EoL). ISO standards allow the calculation of the biogenic carbon removal and requests a separate emissions calculation depending on the application, the time frame of using the carbon etc. Long term uses or other uses in the end-of-life scenario can be considered specifically.

According to ISO 14067 [ISO 14067: 2018], biogenic removals from CO_2 uptake during biomass growth shall be included in the PCF calculation. Removals of CO_2 into biomass shall be characterized in the PCF calculation as –1 kg CO_2e/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]. For more details see chapter 5.2.10.1.

For short term uses of materials with incineration, both approaches are identical in cradle-to-grave considerations. For long term applications, significant differences will be calculated, depending on the final disposal. The effect of the timing of CO_2 emissions and removals shall be assessed. For other technologies that remove CO_2 from the atmosphere, in general these rules apply as well and the specific benefit to the GHG reduction shall be addressed.

Where CO_2 emissions (and upfront removals) arising from embedded carbon of the product in question during the use phase and/or at the end-of-life occur over a longer period of time that still needs to be defined (if not otherwise specified in the relevant PCR) after the product has been brought into use, these emissions can be neglected or can be treated as carbon sinks for longer time periods. For permanent storage, the time frame is 100 years, but any leakages have to be identified, monitored, reported and considered in the PCF calculation of the product. The timeframe of these CO_2 emissions relative to the year of production of the product shall be specified in the life cycle inventory. The effect of timing of the CO_2 emissions and removals from the product system, if calculated, shall be documented separately in the inventory [ISO 14067: 2018].

4.6.6.2 Biogenic emissions in Corporate Accounting

Emissions from biomass sources are typically compensated for by CO_2 absorbed during photosynthesis. Therefore, many companies report zero emissions related to the combustion of biomass. Inconsistencies or confusion may arise if different companies apply different methods or formats to report emissions from biogenic origin [WBCSD (2013)].

According to the GHG Protocol Corporate Standard, biogenic CO_2 emissions (e.g., CO_2 from the combustion of biomass) that occur in the reporting company's value chain are required to be included in the public report, but reported separately from Scope 3.

The requirement to report biogenic CO_2 emissions separately refers to CO_2 emissions from combustion or biodegradation of biomass only, not to emissions of any other GHGs (e.g., CH_4 and N_2O), or to any GHG emissions that occur in the life cycle of biomass other than from combustion or biodegradation (e.g., GHG emissions from processing or transporting biomass).

Scope 1, Scope 2, and Scope 3 inventories include only emissions, not removals. Any removals (e.g., biological GHG sequestration) may be reported separately from the Scopes [WBCSD (2013)].

Within the corporate report the following information might be reported:

- Total Scope 3 emissions excluding any biogenic CO_2 emissions or removals (mandatory).
- Separately: Any biogenic CO_2 emissions (mandatory).
- Separately: Any biogenic CO_2 removals e.g. biological CO_2 sequestration (mandatory).

4.6.7 Market instruments in Scope 3 GHG accounting

Market-based GHG accounting instruments play an increasing role in mitigating Scope 3 emissions within corporate and product GHG accounting. While the current GHG Protocol does not formally endorse Scope 3 market-based strategies like those utilized in Scope 2, amendments are anticipated that will bridge this discrepancy. The GHG Protocol's "Market-based Accounting Approaches Survey Memo" provides the following initial definition of market instruments:

1. Chain-of-custody models, where environmental attributes are transferred across the supply chain via mechanisms like mass-balance or book & claim certificates.

2. Value chain interventions that aim to reduce emissions within a company's primary sourcing regions.

3. Project-based credits, such as carbon offsets or insets.

Some relevant market-based accounting mechanisms for corporate Scope 3 accounting are discussed below:

4.6.7.1 Chain of custody models

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]. There are multiple chain of custody mechanism explained in ISO 22095 standard. Two of the chain of custody methods that are relevant for chemicals value chain Scope 3 accounting are discussed below. In some cases, e.g. EPD programms, it may not be permitted to use these approaches.

4.6.7.1.1 Mass-balance

The GHG Protocol defines mass-balance market instruments as "purchases of certificates in which materials or products with a set of specified characteristics are mixed with materials or products without that set of characteristics."

The mass balance approach is a chain of custody model in which materials with a set of specific characteristics (such as recycled content, bio-content, low emission raw materials, other sustainability attributes as defined in chapter 5.2.8.1) may be mixed according to defined criteria with materials without that set of characteristics (such as virgin fossil materials). In the chemical industry, mass balance chain of custody helps enable fossil raw materials to be replaced by more sustainable alternative materials to reduce the consumption of fossil resources and to transition to a more circular economy.

Under a mass balance chain of custody system, the quantity of certified alternative raw materials can be attributed to a specific quantity of individual products (after adjusting for conversion factors and process yield losses). In contrast to a segregated use of alternative raw materials, mass balance enables to use existing production networks with minimized or no investments into new process technologies and production facilities. According to ISO 22095, a connection between administrative document flow and the physical flow of materials and products must be given in a mass balance approach.

In this document, the Chapter 5.2.10.5 gives guideline for calculating the PCF for mass balance calculations.

Note: The term "mass balance" in these guidelines refers to the chain of custody system, which is different than the concept of physical conservation of mass.

For a meaningful application, a reliable bookkeeping system must be installed to avoid double-counting and the sales of a greater amount of alternative attributed products than possible by the amount of purchased alternative raw materials. In addition, a mass balance approach can also be applied for recycled materials input as feedstocks to the chemicals industry.

4.6.7.1.2 Calculation of mass-balanced products

Mass balance is used in multiple industries in which it is not practical to maintain physical segregation of sustainable and conventional materials during processing. The mass balance approach ensures that the quantity of sustainable production in a supply chain is balanced with (does not exceed) the input of sustainable material and is appropriately adjusted for yields and conversion factors.

Co-processing of sustainable and conventional raw materials results in the production of materials of mixed origin (such as fossil-based, bio-based, recycled waste-based) which are not distinguishable in terms of composition or technical properties. Mass balance allows sustainable content to be attributed to individual outputs to create value from the use of sustainable inputs.

The PCF for mass-balanced products is calculated by replacing the impact of the fossil raw material with the amount that is exchanged by the alternative raw material. Double-counting of the alternative raw material must be avoided. If the alternative raw material is allocated to dedicated mass balance products, all other products shall be calculated with the fossil raw material impact. Furthermore, it shall be technically or chemically possible to produce the mass-balanced product from the alternative feedstock.

4.6.7.2 Book-and-claim

The GHG Protocol Market-based Accounting Approaches Survey Memo defines book-and-claim as "the purchases of certificates in which environmental attributes are separated from the products the company physically consumes." Examples of these systems include programs like low-carbon fuel certificates from logistics suppliers or unbundled Renewable Energy Certificates.

4.6.7.3 Value chain intervention

The GHG Protocol defines value chain intervention as "projects/interventions that reduce emissions or increase removals inside the reporting company's supply shed or sourcing area and are accounted for using Scope 3 inventory methods (e.g., using emission factors derived from primary data specific to individual suppliers that implement interventions). The ISO Standard 14068 on Carbon neutrality can be considered here as well.

4.6.7.4 Project-based crediting

The GHG Protocol defines project credits as: "quantified mitigation outcomes of projects or broader interventions which are credited for GHG claims to be transferred between entities. Credits are quantified using project-based accounting methods in which emission reductions or removals resulting from projects or interventions are quantified relative to counterfactual baseline scenarios." Project-based accounting methods such as ISO14064-2 and GHG Protocol for Project Accounting provide standardization for quantification, monitoring and reporting of activities intended to cause greenhouse gas (GHG) emission reductions or removal enhancements, which is then converted to tradable certificates known as carbon credits (also called offsets). ISO14068-1 carbon neutrality standard specifies principles, requirements and guidance for achieving and demonstrating carbon neutrality through the quantification, reduction and offsetting of the carbon footprint.

Specific rules are applied for carbon credits (offsets). There is a direct or indirect removal included as one process step, often out of the boundaries of the reporting company. In general, the following aspects shall be considered:

- Following the guidance in the GHG Protocol Corporate Standard, the reporting company shall report all offsets separately from their Scope 1, 2 and 3 emissions. This includes both offsets with certificates and without.
- All regulatory reporting requirements must be met.
- Companies shall transparently disclose the origin of reported offsets, including the scheme under which they were generated.
- If a company sells certificates it received for emission reductions realized within its reporting boundaries, it shall report an "offset" with a positive impact. [ISO 14064:2019, WBCSD (2013)].
- Companies may add offsets or other types of carbon credits together if they originate from the same GHG scheme and are of appropriate vintage.

4.6.7.5 Further guidance on market instruments in Scope 3

As the landscape of GHG accounting continues to evolve, the TfS Guidelines may be revised to maintain alignment with the GHG Protocol and other emerging methodologies. Companies are encouraged to stay informed of these developments to ensure that their use of market instruments remains compliant with the latest standards. Recently, ISO 14068 on Carbon neutrality was published and can be considerd accordingly. Until there is further clarity from the GHG Protocol, organizations are recommended to follow these principles when using market instruments in corporate Scope 3 calculation and reporting:

- Participate exclusively in programs with stringent credibility, transparency, and comprehensive documentation.
- Maintain accounting practices that are transparent and in alignment with the GHG Protocol or other applicable standards.
- Gather conclusive evidence that validates the proper implementation of the market instrument.
- Authenticate and quantify the environmental advantages obtained through market instruments, preferably substantiated by certification.
- Explicitly document carbon offsets; these should remain distinct and not be deducted from the organization's inventory of direct or indirect emissions.

05 Specifications for Suppliers’ Product Carbon Footprint Calculation

Product-level CO_2 transparency along the value chain is crucial to identify, track, and reduce greenhouse gas (GHG) emissions in cooperation with supply chain members.

This transparency is increasingly demanded by customers from all industrial sectors who are strongly and increasingly targeting the reduction of GHG emissions.

The sharing of Product Carbon Footprints (PCF) information between supply chain members enables companies to track their Scope 3 GHG emissions and facilitate reduction efforts [GHG Protocol Scope 3 Standard (2011)].

The following requirements apply to the calculation of product-related cradle-to-gate GHG inventories and serve as a global standard/guideline for calculating PCFs in the chemical industry. Adhering to these requirements enables comparability in PCF calculations and hence a level playing field. To create greater transparency and enable comparability, information on the exact methods or standards applied shall be shared downstream as part of the elements for data exchange.

The guideline is applicable to all chemical products, independent of their final use.

PCFs are modelled according to comparative guidelines/ standards, providing consistency in how the results have been modelled. The PCF result between two comparable materials may differ because of differences in technologies, data used from suppliers, geographical aspects, etc.

However, the basis for the modeling should be well described and related to guidelines such as this one to avoid differences that come from using different assessment approaches. The calculation of results should be linked to a meaningful and harmonized reporting that explains in which way the calculations were executed and on which basis the results were generated, specifically in cases of the application of a variety of different methods. Furthermore, the calculation basis, specifically in cases of the application of a variety of different approaches shall follow this guideline. The practitioner or the persons in charge of the creation of the PCF are responsible for the preparation, calculation, quality, and the reporting of the PCF to a third party.

The calculation is only auditable if the reporting is done by the supplier accurately. Therefore, TfS has published the **TfS Data Model** to enable data exchanges via specific platforms and to ensure that the recipient gets clear, high quality and meaningful information.

The guideline was prepared by experts of the "Together for Sustainability (TfS)" organization together with testing companies and third-party organizations. It reflects the status quo of the main recognized standards in the world. It was specified by requirements, procedures, assessment approaches for chemicals. The guideline will be updated if significant changes or adaptations are needed due to changes of other generic standards, new aspects that have not been considered so far or new requirements from the market. It will be published after indicating the revision on the TfS webpage with the changes that have been made compared to the previous version. The outdated versions will be stored in an accessible archive of TfS.

TfS recognizes that it is often difficult to compare PCF data of similar products because of the different underlying methodological decisions made in the calculation, uncertainties of data used, different levels of quality of data, differences in regions, technologies etc. However, the application of this guideline aims to reduce the issues to compare PCF of chemicals. In the future, PCFs will be important information sources to support companies in their GHG reduction strategies.

PCF information from suppliers in accordance to a sector-specific guideline will contribute to the transparency along supply chains. A good reporting addressing all relevant information e.g., scope, standards used, PCR applied, data sources used, allocation methods applied, etc. will allow a better understanding of PCF results for chemicals.

The purpose of the PCF study report is to describe the PCF study, including the PCF or the partial PCF, and to demonstrate that the provisions of this document have been met. The PCF results generated by the companies can be used in different ways. The first instance is a B2B exchange of the data with an internal review recommended. Furthermore, the companies can publish PCF results in different ways, where an external review is requested [ISO 14026:2017]. The results and conclusions of the PCF study shall be documented in the PCF study report without bias. The results, data, methods, assumptions, and the life cycle interpretation shall be transparent and presented in sufficient detail to allow the reader to comprehend the complexities and trade-offs inherent in the PCF study [ISO 14067: 2018].

This guideline focusses on all relevant GHGs as defined by the Intergovernmental Panel on Climate Change (IPCC). The relevant GHG emissions and their emission factors are described in detail in 5.2.6.

However, the general principles can be used and applied for chemicals as well, if other environmental impacts beyond GHGs (e.g., air quality, water use, biodiversity) need to be addressed. These questions are becoming a more and more common ask from customers of the chemical industry and a leverage of the same method across impacts can be possible. Further specifications are needed in this context and can be seen as a possible future task resulting in an extension of the guideline.

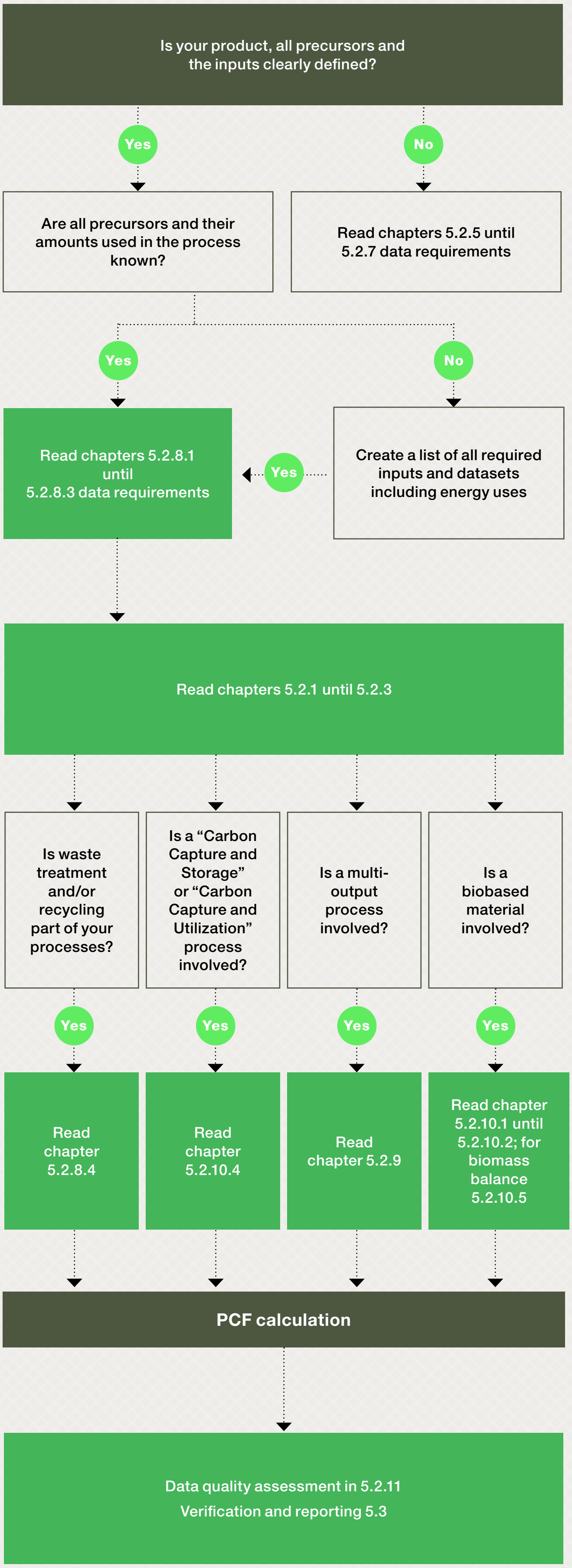
In Figure 5.1 an overview is given for easier navigation in the guideline document and to more easily find the most relevant chapters and skip others. Figure 5.1 should also give support for beginners in this topic to start relatively quick with the first calculations and follow-up with specific questions later if relevant.

TÜV Rheinland Energy & Environment GmbH provided the following services to TfS:

- Assess the guideline against all relevant standards applied (e.g. SBTi, PACT Methodology, GHG Protocol etc.).
- Check if reporting requirements for applicants are sufficiently defined in the guideline.
- Test the level of usability and provide hints for optimization.
- Loops of discussions and potential improvements during testing stage with TfS and finalization stage of the document.

It can been confirmed that the approaches used and the calculation methodology are reasonable, transparent and appropriate for the purpose of the guideline. The presented approach as well as the calculation examples are coherent, transparent and comprehensible.

Figure 5.1 Overview of the main chapters of the guideline



5.1 Goal and Scope

5.1.1 General

The scope of this guideline covers the so-called "cradle-to-gate" approach to calculate a PCF and refers to a "declared unit" (see 5.1.3).

The guideline enables calculating the cradle-to-gate PCF based on standards and guidelines that were developed from different organizations.

General topics follow the standards mentioned in 5.2.4. It is stated, where the guideline defined specific rules for chemicals that are not reflected in detail in the current standards. The guideline is fully compliant with ISO 14067:2018 and the GHG Protocol Product Life Cycle Accounting and Reporting Standard. As a specific requirement, GHG emissions from dLUC and aircraft shall be reported according to the data exchange format if relevant. It is a challenge to be fully compliant with all other standards or guidelines that might be relevant. TÜV Rheinland checked and validated the compliance.

A cradle-to-gate PCF as used throughout this document, is the sum of GHG emissions and removals of one or more selected process(es) in a product system, expressed as CO_2 equivalents (CO_2e) and based on the selected stages or processes within the life cycle. The selected stages in this guideline cover all activities within the defined system boundaries as defined in detail in Chapter 5.1.2.

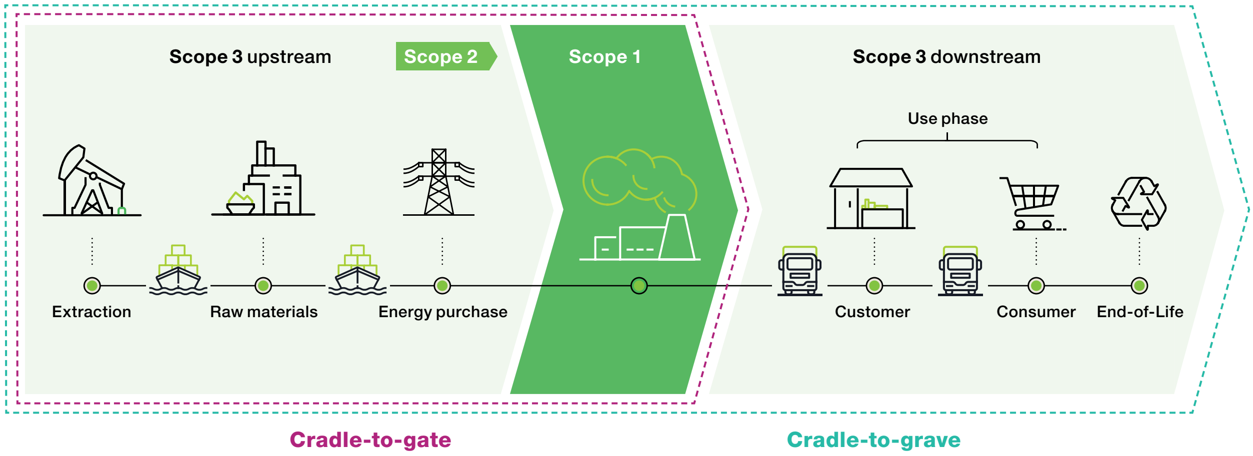
It must be noted that a product assessment limited to only GHGs has the benefit of simplifying the analysis and producing results that can be clearly communicated to stakeholders. The limitation of a GHG-only inventory is that potential trade-offs or co-benefits between environmental impacts can be missed. 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)].

5.1.2 System boundaries

The boundary of the guideline is a cradle-to-gate PCF, comprising all processes of extraction, manufacturing, and transportation, until the product leaves the factory gate. Downstream emissions from product use and end-of-life are in general excluded from a cradle-to-gate PCF (Figure 5.2).

The following activities **shall be included** in a cradle-to-gate PCF calculation: all product related direct (Scope 1) and indirect (Scope 2) GHG emissions of the production process, including fossil or biogenic removals, energy consumption (Scope 2: electricity, external heat and steam; Scope 1: fuel consumption like natural gas, biogas), utilities, manufacturing, inbound transportation, site-to-site transportation, treatment of process waste and wastewater treatment and all Scope 3 related GHG 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.

Figure 5.2 System boundary definition



As the guidance is product-related, the following activities **shall not be included** within the boundaries of a cradle-to-gate PCF: 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. [PACT Methodology], Table 5.1. For renewable energy infrastructure, the equipment especially for solar and wind should be included in the PCF. In solar cells and in wind turbines most of the emissions are coming from the production and should be included in the PCF calculation if the energy consumption is relevant. Please also see Chapter 5.2.3 on requirements to cut off activities.

The following activities should be included or excluded in the system boundary depending on cut-off criteria or customer requirements: Outbound transportation of the product is in general excluded (see Figure 5.2). If outbound transportation needs to be considered by customers' requests, it may be calculated and reported separately. Packaging of the product in question should be included. For many chemicals, the contribution of packaging to the PCF 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).

The system boundary shall be the basis used to determine which unit processes are included within the PCF study. Where PCF Product category rules (PCR) are used, their requirements on the processes to be included supersede those indicated above (see 5.2.4). According to ISO 14067 [ISO 14067: 2018], a PCR is a "…set of specific rules, requirements and guidelines for carbon footprint of a product or partial carbon footprint of a product quantification and communication for one or more product categories". The criteria, e.g., cut-off criteria (5.2.3), used in establishing the system boundary shall be identified and documented internally in the PCF calculation report.

Decisions shall be made regarding which unit processes to include in the PCF study and to which level of detail these unit processes shall be analyzed. The exclusion of life cycle stages, processes, inputs, or outputs is only permitted if they do not significantly change the overall conclusions of the PCF calculation. In a "cradle to gate" approach, the use and disposal phases are not always of minor relevance but are not in the scope of the analysis and are excluded. In Chapter 5.1.3 the cut-off approach is described in detail.

The following Table 5.1 describes generically the activities that shall be included or excluded from the system boundaries as well as the ones that are optional.

5.1.3 Declared Unit (DU) of PCF

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 PCF. In case of chemical products, the declared unit is often defined as 1 kg of product.

This TfS guideline deals exclusively with the use of a Declared Unit as it only guides in calculating cradle-to-gate PCFs and thus does not include the full product life cycle.

The PCF, expressed in kg CO_2 equivalents per Declared Unit, reflects the cumulated climate change impact of air emissions of greenhouse gases (GHGs). Every supplier of the same product shall calculate its emissions using the same Declared Unit [BASF SE 2021].

Standard unit should be kg CO_2 equivalents per kg product preferably. For some specific products like gases (e.g., Hydrogen, LPG) the PCF might be expressed per unit norm cubic meter of product. Furthermore, some products are sold based on a volume unit (like liter), or pieces (e.g.: automotive parts) and in that case the PCF may be expressed in the respective unit. In these cases,

Table 5.1 Activities to be included and excluded in the system boundaries and optional activities

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.

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 TfS Data Model. Any other unit of measurement like Euro shall not be used.

For processes, the PCF may be expressed as kg CO_2e 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 PCF linked to the Declared Unit should be reported as kg CO_2 equivalents per Declared Unit with one decimal. More decimals are not meaningful due to the variability of the figures. Results with a second decimal should be rounded: In the case of a high value of a PCF, a decimal can be omitted, in case of very low PCF more decimals than one decimal can be meaningful.

1.25 kg are rounded to 1.3 kg CO_2 equivalents; 1.24 kg are rounded to 1.2 kg CO_2 equivalents.

A PCF study shall **clearly specify** the Declared Unit of the system under study. The Declared Unit shall be **consistent with the goal and scope** of the PCF study [ISO 14067: 2018]. 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 PCF 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 factory gate. 1kg refers only to the product mass. The packaged product will weigh more than 1 kg.

$$\frac{\text{kgCO}_2\text{e product (including packaging impact)}}{\text{kg product (excluding the mass of packaging)}}$$

TfS will consider specific guidance for the inclusion of packaging in the next revision of the guideline.

In all cases, a clear definition of the **Declared Unit** as basis for the PCF shall be disclosed. The calculations shall refer to the **Declared Unit** and shall be integrated in the deliverables when PCF data are exchanged between companies.

5.2 Calculation rules

5.2.1 Steps of PCF calculation

This chapter comprises the key calculation criteria to be followed while developing PCFs.

A PCF study in accordance with this document generally goes through the four phases of Life Cycle Assessment, resulting in the following general steps:

(i) Goal and scope definition: The declared unit shall be defined and all relevant activities and processes within the system boundaries identified. The system boundaries are outlined in chapter 5.1.2 and comprise all service, material and energy flows that become, make, and carry the product from raw material extraction to the factory gate.

(ii) Creating the Life cycle inventory by collecting activity data: Activity data shall be collected for processes within the system boundaries (e.g. material input, energy inputs such as electricity, cooling and heating, purchased products and direct emissions). The applicable data requirements for the different types of activity data are described in chapter 5.2.8. See chapter 5.2.3 for details on which activities can be excluded from the collected data.

(iii) Life cycle impact assessment:

a. Calculating emissions: GHG emissions arising from a process shall then be calculated by multiplying the relevant activity data with its respective emission factor (CO_2e per declared unit). The term activity data describes e.g. the input of materials, a process, a chemical reaction, a work up or purification step.
Data types and emission factor sources are described in chapters 5.2.5 and 5.2.6.

b. Additional steps can be required such as splitting emissions from multi-output processes or allocating them to different outputs. For guidance on such subjects see chapter 5.2.9.

c. To allow for flexibility in applying accounting standards, calculations should be completed such that different allocation methods could be applied if needed. This ensures that different standard guidelines can be adhered to if required [PACT Methodology], [BASF SE 2021].

(iv) PCF consolidation: The PCF shall then be calculated summing up all GHG emissions.

a. If the company produces the product in several different sites, bottom-up calculations for each production site using site-specific data, and if applicable, country-specific secondary data for processes not under the control of the reporting company, shall be performed. For communication purposes, the company may aggregate the site-specific data into a weighted average based on the production volumes of the respective productions. If site-specific PCF data is averaged, this must be transparently stated. In addition, it will be reflected in a lower data quality score.

b. In general, data collection should be as granular as possible, ideally from the specific processes involved in the production of the product under study. When process level data is not available, the data must be collected at plant or even site level, preferring plant level data to site level data. In these cases, emission factors from energy use or direct GHG emissions from a whole facility or site need to be attributed to the specific processes of the facility or site. This shall be done using a mass, time, or other physical attribution approach. For this a break-down factor (BDF) is needed to attribute the GHG emissions from a facility or a site to the individual process. The BDF is calculated as described above for example as a ratio of the production volume of the facility or entire site (in tons). Subsequently, the GHG emissions of the plant or site are multiplied by this BDF to result in process-level GHG emissions.

(v) Documentation and reporting.

5.2.2 Temporal Scope

The time boundary of a PCF refers to the time period for which the PCF value is considered to be representative [ISO 14067: 2018]. The following time boundaries apply for the different types of data:

- **Primary data** used in the calculation of PCFs 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 PCF 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 atypical 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 a PCF calculation [BASF SE 2021], [PACT Methodology].
- **Secondary data** used for all inputs and outputs should reflect the most recent activity data and/or the latest LCIs available. LCI data (e.g., from databases) used in the calculation of PCFs 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.
- **PCFs** should be calculated on a regular basis to track improvements over time. However, this may pose a challenge for companies that rely on manual PCF calculations for products and who do not have an automated calculation approach. PCFs shall therefore 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 PCF). Companies may update their PCF calculations on **a more regular basis** (e.g., annually). TfS decided that after three years or if the production process has changed significantly, PCF values are no longer considered representative and must be re-calculated. Once a PCF has been revised, the revised version will replace the original PCF and be valid for 3 years.

- The time boundary of the PCF calculation is the reference year. The PCF's **reference year** and date of calculation/publication shall always be disclosed alongside the PCF value.

5.2.3 Criteria to exclude certain activities (Cut-off)

In general, **all processes, flows and activities**, that are attributable to the product system shall be **included** in a PCF (see 5.1.2 on generally excluded and included activities) [BASF SE 2021] [ISO 14067: 2018]. The LCI data collection process shall aim for **completeness**. Where quantitative data are available, they shall be included. However, no undue effort should be spent on developing data of negligible significance concerning GHG emissions. If individual material or energy flows are found to **be insignificant** for the carbon footprint 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 PCF 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 signifcant.

Cut-off criteria specify the amount of material or energy flow or the level of significance of GHG emissions associated with unit processes or the product system that may be excluded from a PCF study [BASF SE 2021]. Furthermore, cut-offs may become necessary in cases where **no data are 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 are available, but elementary flows are significant, data gaps should be closed in accordance with chapters 5.2.6 and 5.2.8.

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 PCF 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 a PCF 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 a PCF 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 impact on the PCF accurately. Where materials are used in a process that are considered or estimated to have a very high PCF, the influence on the overall PCF shall be evaluated and the cut-off kept below 3 % of the PCF.

3. In cases where the input and influence on the PCF is 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. Input material flows of precious metals like platinum group containing catalysts that have a considerable upstream environmental footprint shall be considered in the PCF calculation, regardless of their relative contribution to the total mass of material flows, even if their mass input is < = 1% of the total mass. The PCF calculation should at minimum consider the loss of material (e.g., the loss of catalyst) and assign a PCF 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.

5.2.4 Standards used

5.2.4.1 Generic standards and PCR

This sectorial TfS PCF Guideline 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 guideline follows **ISO 14067: 2018 for Product Carbon footprints (PCF)**. According to ISO 14067 [ISO 14067: 2018], the carbon footprint of a product is the "…sum of GHG emissions and GHG removals in a product system, expressed as CO_2 equivalents and based on a Life Cycle Assessment using the single impact category of climate change." According to ISO 14067 [ISO 14067: 2018], a PCR is a "set of specific rules, requirements, and guidelines for carbon footprint of a product or partial carbon footprint of a product quantification and communication for one or more product categories." It also draws from other guidelines such as the **GHG Protocol** developed in recent years. PACT Methodology and WBCSD Life Cycle Assessments guideline were considered as well. Generally, the guideline follows these standards and provides clarification and examples for the chemical industry.

To increase the consistency of PCF calculations along the value chain the following aligned prioritization hierarchy of guidelines shall be followed for PCF calculations:

1. PCR which was developed based on **TfS PCF Guideline or accepted by TfS**.

2. Product or sector-specific guidelines based on ISO 14000 series (such as PCRs published by Plastics Europe).

3. **TfS PCF Guideline** if a PCR does not exist yet, the guideline can be used to calculate the PCF.

4. ISO 14067 standard [ISO 14067: 2018].

5. PACT Methodology; GHG Protocol Product Standard [GHG Protocol Product Standard].

6. Product Environmental Footprint Category rule (PEFCR) developed under the European Product Environmental Footprint initiative [EU PEF].

If multiple officially declared PCRs for the same product from different organizations exist, TfS will conduct a review with an expert team and declare the “TfS accepted PCR”. As a basis for the decision the application of the TfS PCF Guideline or other relevant standards is firstly checked. Furthermore, TfS publishes and updates every year a list of the “TfS accepted PCRs” in general independently if different PCRs exist. Organizations can submit their PCRs for TfS listing. A defined process will be applied to decide on acceptance. In the case of sector-specific rules which are not officially declared as PCRs or PEFCRs, application shall also be justified and verified by TfS.

In the non-exhaustive list, the date of the document and the date of the final review of TfS will be added to avoid the automated acceptance of updated documents that TfS was not aware of and did not review. The list can be found here: **https://www.tfs-initiative.com/pcf-guideline#multioutputprocessesand acceptedpcrs**

5.2.4.2 Process of PCR acceptance and listing

Organizations that want to have their PCRs accepted and added to the PCR list shall submit the PCR and other explanations to TfS for review. TfS checks whether all requirements are met for the PCR to be recognized and to achieve the “TfS accepted PCR” level. All PCRs with a focus on chemicals that are not governed by regional laws or regulations can be reviewed and approved for inclusion in the official and publicly available TfS list. The expert team checks if the main requirements from ISO/TS 14027:2017 Environmental labels and declarations — Development of product category rules are fulfilled. In addition, the PCR shall include all applicable requirements for conducting the LCA according to ISO 14044, ISO 14046, ISO 14067 and the TfS PCF Guideline, including but not limited to:

a) the functional or declared unit;
b) the system boundary: the definition of the system boundary shall follow the requirements of ISO 14044:2006, 4.2.3.3;
c) reference to any specific data or calculation rules to be used in the calculation;
d) allocation rules: the PCR shall define the allocation rules in accordance with ISO 14044:2006, 4.3.4.

The PCR review shall address at a minimum:

a) general information on the PCR (initiator, programme operator, registration code or other identifier);
b) scope of the PCR and definition of the product category or product categories addressed;
c) other standards applied for the product category, that are relevant to the PCR review;
d) critical evaluation of LCA-related requirements of the PCR with respect to the functional unit or declared unit;
e) system boundary;
f) life cycle inventory analysis, such as the methods of allocation, data quality requirements, electricity modelling;
g) life cycle impact assessment;
h) life cycle interpretation;
i) assumptions and limitations of the LCA calculation rules;
j) choice of indicators if relevant (the TfS PCF Guideline focusses on GHG emissions);
k) data source and quality requirements;
l) documentation of the declared technical information on life cycle stages that have not been considered in the LCA of the product, (e.g. transport distances, product lifetime, energy consumption during use, maintenance cycles);

The PCR document shall transparently report on:

a) notification of the representatives of the interested parties in the development of the PCR and the formation of the PCR committee and their interest to be implemented in the PCR
b) PCR committee is this set-up by the interested parties
c) check the balance of the mix of interested party perspectives and competencies (see ISO 14025:2006, 5.5, 6.5 and 9.3). If an interested party was excluded, this shall be justified;
d) check that the PCR committee chair had sufficient knowledge of and proficiency in LCA and environmental product declarations according to ISO 14025 and footprint communications based on ISO 14044, 14025, ISO 14046 and ISO/ 14067, TfS PCF Guideline;
e) make publicly available the PCR committee’s decisions regarding any submitted comments.

If different officially declared PCRs for the same product from different organizations exist, TfS will review them with an expert team and declare one of these PCRs as the “TfS accepted PCR”. As a basis for the decision the coherence of the TfS PCF Guideline will be checked.

In the TfS decision process, priority shall be given to allocations rules accepted by TfS in a published list or PCR given in:

1. Existing regional law or regulation.
2. PCRs from worldwide operating associations.
3. PCRs from regionally operating associations (e.g., Plastics Europe).
4. PCR from EPD programs.

At least every year TfS publishes and updates a list of the "TfS accepted PCRs". In the case of sector-specific rules which are not officially declared as PCRs or PEFCRs, application shall also be justified and verified by TfS.

In the process TfS will consider the intention of a PCR as well submitted with the following criteria:

1. If the calculation is to be done for compliance purposes, PCRs aligned to existing regional law or regulation should be followed (e.g., PEFCRs)
2. If the calculation is to be done for commercial purposes, companies should follow a world-wide valid PCR, If they are not available they can follow regional PCR applicable to the given geography of the market.
3. If the intended market is unclear, companies should prioritize more inclusive PCRs to favor broader acceptance.

5.2.5 Data types and sources

Data can have different levels of quality. Every PCF 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 EU-ETS. 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 PCF. For share of primary data and data quality rating, please refer to chapter 5.2.11.

The most recent databases at point of calculation should be used. E.g. there was a significant change in the datasets in 2023/2024 connected to increased methane emissions from the extraction processes of oil and gas. As a consequence, the database versions ecoinvent V3.10, Sphera MLC 2024.1 or Carbon Minds cm.chemicals database Version 2.00, July 2023, or later versions of these databases, should be used if datasets for these secondary data providers are used in the PCF calculations. Other data sources and supplier PCFs should also be updated for the same reasons and as there is a high likelihood that they are using the same databases for the PCF calculations.

Sources can be defined as:

Primary data:

- Company-specific data – refers to directly measured or collected data from one or more processes (process-specific data), from one or more facilities (facility- or plant-specific data) or from one or more sites (site-specific data) that are representative of the activities of the company (company is used as synonym of organization). To determine the level of representativeness a sampling procedure may be applied[1].
- Primary data are defined as data from specific processes in the studied product's life cycle. They are collected for all processes under the ownership or control of the reporting company. Direct emissions data, emission factors and process activity data can be classified as primary data if they meet the definition.
- In general, primary, company-specific data should be collected and calculated as far as possible, i.e., at the highest level of granularity. This means that process-specific data is preferred over facility-specific data which is preferred over site-specific data.
- If only facility-specific or site-specific data of a company are available, they shall be collected or calculated and shall be representative of the facility or site for which they are collected.
- Facility or site-specific data shall then be broken down to the product level based on mass or other meaningful relations.
- Site-specific data should also be used for those unit processes that are commonly used for several processes, e.g. incineration or waste treatment. The overall consumption data should be calculated per service unit, e.g. kg CO_2e per ton of waste incinerated. In addition, available information on specific emissions in specific processes shall be considered (e.g. SF_6 emissions from an incineration process of plasma that is used in the semiconductor industry).

Several standards prioritize the use of primary data, which is supported by this standard as well, if the data quality is high (see 5.2.11).

Secondary data:

- Secondary data – Defined as data that are not directly collected, measured, or calculated based on specific production data available for the company. Secondary data can include supplier and technological specific data derived from detailed data at plant/site level from market reports or patents, industry average data, or literature studies and can be an important and meaningful source for data included in PCF calculations.
- Secondary data includes industry averages, estimates based on literature studies, associations, published production data, government statistics, literature studies, engineering studies and patents and may also be based on financial data. It can contain proxy data generated by external expert judgement and other generic data. In addition, it can be sourced from a third party LCI database, open sources, PCF calculations, etc.
- It can be independently reviewed which increases the reliability and Data Quality Rating (DQR) score. Secondary data shall only be used for inputs and outputs where the collection of primary data is not practicable, or for processes of minor importance or where secondary for various reasons have a higher quality or fit better than primary data (e.g. association data for specific products).
- Secondary data can have the same level of quality as primary data, depending on the process of generation of the data, of meaningful fit to the data used, the level of aggregation etc.

(1) Please see Appendix A of the GHG Protocol Corporate Standard for more information on sampling and sampling techniques.

In case of 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 following sections give additional guidance on filling data gaps with proxy data and estimated data.

Table 5.2 gives a summary and 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 studied process 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 PCF, using polyethylene data as a proxy for polypropylene might be sufficient as well.
- Adapting an electricity grid emission factor for one region to another region with a different generation mix.
- Customizing a 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 studied product.

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 PCF result. If processes are determined to be insignificant based on estimated data, the process may be excluded from the inventory results (cut-off criteria). Criteria for determining insignificance are outlined in chapter 5.2.3 [GHG Protocol Product Standard]. If the data gap is significant and cannot be closed by the other types of data defined in this chapter, an estimation of the data shall be introduced. This should be done carefully under consideration of all knowledge of the data gap with a subsequent generation of estimated data. The estimated data shall be replaced by primary or secondary data as soon as possible in the update of the PCF. To assist with the data quality assessment, any assumptions made in filling data gaps, along with the anticipated effect on the product inventory results, should be documented [ISO 14067: 2018].

5.2.6 Emission factor requirements and sources

Emission factors are the GHG emissions per unit of activity data, and they are multiplied by activity data to calculate GHG emissions. Emission factors may cover one type of GHG (for example, CH_4/liter of fuel) or they may include many gases in units of CO_2 equivalents. Emission factors can include a single process in a product's life cycle, or they can include multiple processes aggregated together.

Specifications

Table 5.2 Data hierarchy for energy and material inputs regarding primary, secondary and proxy data [PACT Methodology]

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.

Life cycle emission factors that include emissions from all attributable upstream processes of a product are often called cradle-to-gate emission factors. Companies should understand which processes are included in the inventory's emission factors to ensure that all processes in the product's life cycle are accounted for in the data collection process.

Emission factors come from different sources and a distinction is made between primary and secondary emission factors:

Primary emission factors are emission factors calculated based on primary activity data for a process under a company's control or provided by a supplier for a process under their control. If the emission factor for a raw material is provided by a supplier, it is also called supplier-specific data.

Secondary emissions factors are derived from sources such as LCA databases, published product inventory reports, government agencies or industry associations. Secondary or default emission factors are based on secondary activity data. The source of secondary data must be specified in the report.

Emission factors shall always include all GHGs and be cradle-to-gate emission factors that include emissions from all attributable upstream processes of a product.

The following hierarchy shall be applied when selecting emission factors:

1. Where primary emission factors are available directly from raw material and energy suppliers, or internal processes, these shall be used. The quality of the supplier- or company-specific emission factor is to be evaluated and checked for appropriateness (see below: data requirements on primary data or reference to appropriate chapter).

2. When using emission factors from utility companies, e.g., for electricity or steam (so-called market-based factors), it must be ensured that these are cradle-to-gate emission factors, including both, the emissions from combustion as well as the emissions from the provision of primary energy carriers. If the utility company cannot provide a life cycle emission factor, additional information such as the primary energy carriers used, and their respective shares needs to be disclosed. Based on this information, the upstream emissions from the provision of the energy carriers shall be calculated to complement the CO_2 emission factor from combustion to obtain a life cycle emission factor as described under 5.2.8 Activity data requirements. Additionally, the emission factors provided should include all GHGs but at least cover CO_2, which is by far the largest contributor (>95%) to GHG emissions from combustion of primary fuels. The emission factors shall be expressed always as CO_2e.

3. The utility providers should use either the efficiency or energy allocation approach when calculating emissions from Combined Heat and Power (CHP) installations plants, following the recommendations of the WBCSD accounting document which includes efficiency values by defaults to be used if needed [WBCSD Chemicals [2013]].

4. If primary emissions factors are not available, use secondary emission factors that are most suitable according to chapter 5.2.6. Among available data, use PCF values that are most representative and specific to the geography and technology used to produce the raw materials, utilities, and fuels. Only data from high quality and verified databases as listed below should be used as source of secondary data.

Additional requirements for the selection of secondary data for raw material apply as shown below. The following selection hierarchy shall be followed [BASF SE [2021]]:

1. If the production origin (region or country) and production technology of the supplied raw material is known, choose a regional or country/technology specific emission factor. A region can be the whole world, a group of several countries (e.g Europe) or a smaller area (e.g a group of states in the USA, a province in Canada) E.g Hydrogen liquid chlor-alkali electrolysis, membrane cell production in Europe.

2. If the production origin (region or country) of the supplied raw material is known, but the technology is not known, choose a regional or country-specific production mix, e.g Hydrogen liquid production in Europe.

3. If the production origin is not known, choose a regional or country-specific consumption mix based on the location of your direct supplier, e.g Hydrogen liquid market in Europe.

4. If there is no regional or country-specific dataset available choose the same raw material from another country or region which is the most appropriate in terms of GHG emissions. E.g Hydrogen liquid chlor-alkali electrolysis, membrane cell in Europe for a supplier located in Brazil rather than using a global average value based on a high share of countries where the energy is mainly based on coal.

5. If the specific raw material is not available choose an appropriate proxy e.g., a chemical substance from the same chemical group.

Data quality of inbound and inter-site transports is based on primary data from a database for transport activities including emission factors of transport modes with a high quality.

In general, life cycle emission factors shall be sourced from and calculated based on data from verified sources such as listed below (non-exhaustive list):

- Verified data from associations such as ISOPA, Plastics Europe, World Steel association etc.
- LCA databases such as Sphera Managed LCA content (MLC), Ecoinvent, Carbon Minds, Agribalyse, ELCD (PEF), IDEA database, etc.
- Official national emission factor databases such as US EPA, IEA, Defra, etc.
- GLEC Framework [GLEC Framework] or DIN EN ISO 16258 for transportation.

If secondary emission factors are not available within the references listed above, other sources or proxy data may be used to fill in the missing emission factors.

In any case, the source of secondary data or the employment of proxy data sources shall be reported. The extent to which secondary data is used shall be specified in relation to all GHG emissions by CO_2 equivalents.

The sources should be specified as defined in the TfS Data Model or more details on the reporting requirements including the attributes that shall be reported for primary and secondary data as well as for the use of databases of secondary data.

5.2.7 Life Cycle Impact Assessment (LCIA)

A PCF represents the potential life cycle impact of a product in the environmental impact category of climate change. This impact category considers that different GHGs have different impact on climate change, expressed as their global warming potential (GWP) with the unit kg CO_2 equivalents (CO_2e).

The basic equation to calculate GHG emissions (CO_2e) for an activity data is defined in Formula 5.1:

Formula 5.1

Kg CO_2e =	Activity data	X	Emission factor	X	GWP
	Amount of activity		(kg GHG/ activity)		(kg CO_2e/kg GHG)

For example, if the activity is the purchase of 5000 kg of methanol as a raw material and the supplier-specific emission factor is 0.80 kg CO_2e/kg, then the GHG emissions for the activity 5000 * 0.80 = 4000 kg CO_2e.

The basic equation to calculate CO_2e for a direct emission is defined in Formula 5.2:

Formula 5.2

Kg CO_2e =	Direct emission Data	* GWP
(unit)	(unit) (kg GHG)	(kg CO_2e/kg GHG)

The types of emission factors needed depend on the types of activity data collected.

In Figure 5.4, an example is described for the Chlor-alkali electrolysis gate-to-gate process data. The chlorine production weighted average of selected material and energy inputs and outputs are shown per kg chlorine. The values in the figure do not represent allocated but total in- and outputs of the average electrolysis process divided by the chlorine amount produced and just show only some inputs.

The allocation follows the generation of this GHG information. It is shown, how activity data and emission factors shall be introduced to generate a guideline compliant data set prior to allocation [EUROCHLOR 2022].

Figure 5.3 Types of data for PCF calculation on the example of production of 1 kWh of electricity

ACTIVITY DATA	DEVELOPING EMISSIONS INVENTORY PER ACTIVITY		CALCULATION OF EMISSION INVENTORY WITH ACTIVITY DATA	EMISSION FACTOR PER GHG	LIFE CYCLE IMPACT ASSESSMENT WITH GLOBAL WARMING POTENTIAL (GWP)-FACTORS	GHG EMISSION FACTORS / PCF DATA	
Purchase of oil	Dataset from supplier (TfS) cradle-to-gate PCF: PCF / kg oil	X	0.5 kg oil	0.2 kg CO_2/kg	1 kg CO_2e/kg CO_2	0.1 kg CO_2e/kWh	1.13 kg CO_2e/kWh
Transport of oil via truck	Dataset from LCA database cradle-to-gate LCI: GHG LCI / kg*km	X	0.5 kg oil (120 km transport)	0.2 kg CO_2/ t*km 0.01 kg CH_4/ t*km	1 kg CO_2e/kg CO_2 30 kg CO_2e/kg CH_4	0.03 kg CO_2e/kWh	
Combustion of oil in generator	Calculation of GHG emission based on stoichiometry: GHG LCI / kg oil	X	0.5 kg oil	2 kg CO_2/kg	1 kg CO_2e/kg CO_2	1 kg CO_2e/kWh	
List of activities within system boundary to produce the product	Different sources for emission factors are available		Per declared unit 1 kWh	Inventory of GHG emissions per impact contribution	GWP-factors translate individual GHG into the common unit CO_2e	Aggregated GHG emissions in CO_2e per declared unit	

Figure 5.4 Chlor-alkali electrolysis gate-to-gate process data of data for PCF calculation and transfer into a basic PCF prior to allocation

ACTIVITY DATA	DEVELOPING EMISSIONS INVENTORY PER ACTIVITY		CALCULATION OF EMISSION INVENTORY WITH ACTIVITY DATA	EMISSION FACTOR PER GHG	LIFE CYCLE IMPACT ASSESSMENT WITH GLOBAL WARMING POTENTIAL (GWP)-FACTORS	GHG EMISSION FACTORS / PCF DATA	
Using grid electricity	Calculation of GHG emission based on data from grid: GHG LCI / kWh	X	2.36 kWh	CO_2 0.395 kg CO_2 / kWh	CO_2 1 kg CO_2e / kg CO_2	CO_2 0.93 kg CO_2e / kg	
Purchase of salt	Dataset from supplier (TfS) cradle-to-gate PCF: PCF / kg oil	X	2.15 kg salt	CO_2 0.2 kg CO_2 / kg	CO_2 1 kg CO_2e / kg CO_2	CO_2 0.43 kg CO_2e / kg	CO_2 1.4 kg CO_2e / kg
Purchase of sulphuric acid	Dataset from LCA database cradle-to-gate LCI: GHG LCI / kg	X	0.01 kg sulphuric acid	CO_2 0.14 kg CO_2 / kg	CO_2 1 kg CO_2e / kg CO_2	CO_2 0.001 kg CO_2e / kg	
List of activities within system boundary to produce the product	Different sources for emission factors are available		Per declared unit 1 kg Chlorine	Inventory of GHG emission per impact contribution	GWP-factors translate individual GHG into the common unit CO_2e	Aggregated GHG emissions in CO_2e per declared unit	

The PCF calculation consists of the sum of each GHG released and removed from the product system and application of allocation rules when necessary (see chapters 5.2.9 and 5.2.10).

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.

The AR 6 GWP-100 characterization factors **shall be extracted in priority from Table 7.15** of Chapter 7 of the IPCC AR6 Climate Change 2021 Physical Science Basis. This table includes the chemical effects of CH_4 and N_2O [IPCC 2021- The Physical Science].

The AR 6 GWP-100 characterization factors for the substances that are not listed in the Table 7.15 shall be extracted from **Table 7.SM.7** in the Chapter 7 Supplementary Materials of the AR6 Climate Change 2021 Physical Science Basis [IPCC 2021- The Supplementary Material].

All PCFs shall be consistently calculated with the 100-year GWP characterization factors according to IPCC's Sixth Assessment Report AR 6 [IPCC, (2021a), Climate Change 2021- The Physical Science Basis]. Any supplier PCF data that is calculated in AR5 can be used during a transition period until end of 2024.

The PCF report shall disclose which IPCC Assessment Report basis is used.

5.2.8 Activity data requirements

Activity data describe specific applications and uses of materials, energies, services etc. In an LCA the description of activities within a system boundary is needed to generate mass flows of materials uses, energy uses, etc. The amounts of the activities are later linked with life cycle inventories to calculate the contribution of this activity to the PCF of the whole product.

5.2.8.1 Electricity and thermal energy

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 GHG 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).
- GHG emissions **during 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).

For sources of emission factors see chapter 5.2.6. If sources such as IEA or EPA are used, it shall be ensured that emissions associated with upstream activities are also included.

A company may purchase primary energy carriers such as natural gas, oil or coal either as a raw material for further material processing or as fuel to generate energy. The upstream emissions from activity to provide these primary energy carriers shall be estimated as described in chapter 5.2.8.2. Raw materials.

Thermal energy: Steam, heat and cooling systems

Companies shall report emissions from the purchase and use of these energy products the same as for electricity: according to a location-based and market-based method if the contractual instruments used meet the Scope 2 Quality Criteria as appropriate for gas transactions.

Self-generated thermal energy

If the energy is internally generated (e.g. on site) and consumed for the production of the studied product, the primary data of the energy generation system shall be used to calculate the PCF of the product. Primary data for both, activity data and direct emissions shall be collected via a bottom-up approach.

Thermal energy may also be generated as a co-product of a chemical process (e.g. excess steam). See chapter 5.2.9 for further guidance on how to account for emissions from energy and other co-products.

Purchased thermal energy

If the reporting company purchases thermal energy, GHG emission factors from a supplier-specific energy product shall be used (market-based approach).

A market-based method reflects emissions from electricity that companies have purposefully chosen (or their lack of choice). It derives emission factors from contractual instruments, which include any type of contract between two parties for the sale and purchase of energy bundled with attributes about the energy generation, or for unbundled attribute claims.

If the utility provider is not able to provide a life cycle based GHG emission factor for the energy product but only the CO_2e emission factor from direct emissions (e.g. combustion), the upstream emissions for the fuels that go into the energy production need to be added. In this case, the energy provider needs to provide information on the primary energy carriers used and their share. The GHG emission factors shall be rated with a DQR assessment following this standard.

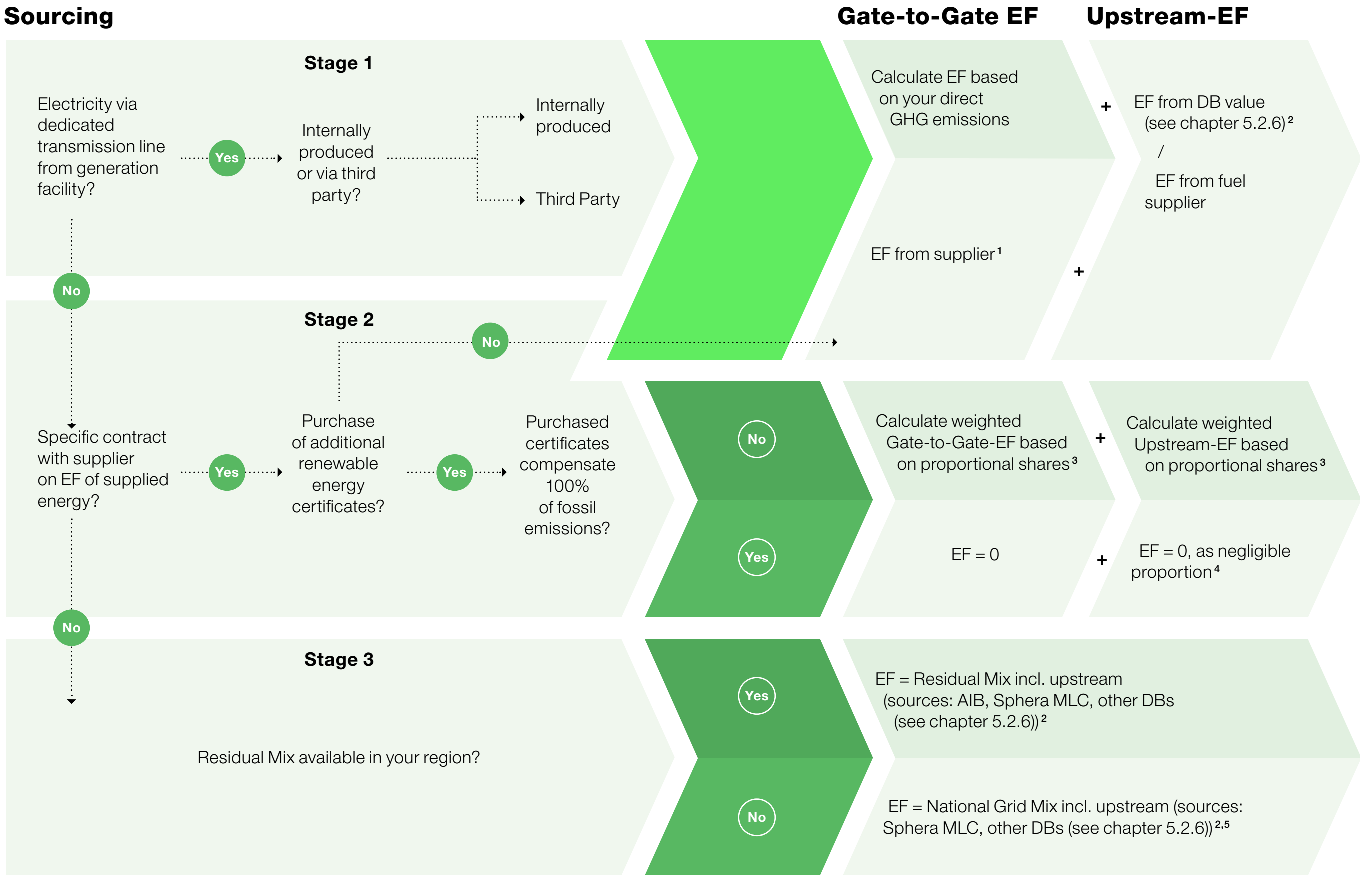
Electricity

For the use in the PCF calculation organizations should generally calculate the emissions of electricity following the market-based approach (as described in the GHG Protocol Scope 2 Guidance). The electricity accounting approach used should be addressed in the PCF reporting. Please follow the decision tree in Figure 5.4 to determine your options on GHG emissions of procured electricity. As stated above the total GHG emission factor should include GHG emissions during generation of the electricity (gate-to-gate) and upstream emissions from the primary energy supply system. For convenience it is possible to add both factors to result a total GHG factor if both refer to the same energy unit. The decision tree is divided into three stages.

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 in stage 3 (see Figure 5.4).

Gate-to-gate emission factors consider emissions within the company boundary excluding all upstream emissions.

Figure 5.5 Decision tree on selection of proper emission factors for externally sourced electricity



(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.

Stage 1: Check if electricity is via a dedicated transmission line from the generation facility

Determining the gate-to-gate emission factor

If there is a dedicated transmission line between the organization and the electricity generation plant and no certificates (also known as contractual instruments) for that consumed electricity have been sold to a third party, GHG emission factors from the supplier-specific electricity shall be used.

- If the electricity is internally generated (e.g. on-site generated electricity) primary data of the electricity generation system shall be used to calculate the PCF of the product.
- If the electricity is provided by a third party, a GHG emission factor obtained from the third party may be used.

If there is a dedicated transmission line between the organization and the electricity generation plant and energy attribute certificates have been sold by contractual instruments to a third party, then the organization must start in stage 3 of the decision tree.

Determining the upstream emission factor

The GHG emissions occurring during the generation of the electricity are included in the calculation of the supplier-specific emissions factor. Additional upstream GHG emissions (e. g. from mining and transport of fuels to the electricity generation facility) and potential T&D losses can either be requested from the suppliers of fuel or electricity or calculated from database values (suitable databases see chapter 5.2.6). If the organization has internally produced electricity and decides to calculate upstream GHG emissions from database values, the fuel consumption per unit of electricity produced serves as a basis. In case of electricity from third parties the composition of the electricity mix is required for calculation.

Stage 2: Electricity from the grid (specific contract with supplier on energy mix)

Determining the gate-to-gate emission factor

If the organization has a specific contract with an electricity supplier regarding electricity with a certain GHG emission factor, be it exclusively for renewable energy such as a PPA or a (partial) fossil-based electricity, and no further renewable energy attribute certificates are purchased, then the organization shall use the emissions factor for the supplier-specific electricity product. If this emission factor is not available, then the emission factor representing the total electricity portfolio of the supplier can be used.

In the case that unbundled renewable energy certificates are purchased, the organization must check if they are sufficient to cover the fossil emissions of the obtained electricity. If not, then a proportional gate-to-gate emission factor for the electricity shall be calculated based on the remaining share that is not covered by the certificates (see footnote (3) in Figure 5.5) or a mass balance approach shall be applied (see further notes on renewable electricity in this chapter). If the certificates compensate the fossil emissions, the gate-to-gate emission factor can be set to zero.

Minimum criteria regarding reliability should be considered when purchasing renewable energy certificates such as the unique claim, age of the RE generation plant since, as very old certificates are seen critical or additionality. The ALCA guidance can be used as a guidance where RE100 addresses the age of the site but does not consider a synchronous mode of the power generation (**https://aclca.org/wp-content/uploads/2022-ACLCA-PCR-Open-Standard_Addendum_Quantifying-Renewable-Electricity-Instruments-in-EPDs_FINAL_061323.pdf**).

Please note that via contract the electricity supplier must guarantee that their product is tracked to ensure that no double-counting of renewable electricity occurs.

Determining the upstream emission factor

Additional upstream GHG emissions (e. g. from mining and transport of fuels to the electricity generation facility) and potential T&D losses can either be requested from the suppliers of electricity or calculated from database values (suitable databases see chapter 5.2.6). If the organization decides to calculate upstream GHG emissions from database values, the composition of the electricity mix is required for calculation.

In the case that further renewable energy certificates are purchased, the organization must check if they are sufficient to cover the fossil emissions of the obtained electricity. If not, a proportional upstream emission factor for the electricity must be calculated based on the remaining share that is not covered by the certificates. If the certificates compensate the fossil emissions in the gate-to-gate factor, the organization should determine the upstream emissions of the applied renewable energy type by calculation from database values. The upstream emissions may be neglected if they are insignificant and thus fall under the cut-off criteria (see chapter 5.2.3). To verify that, primary data should be used. If they are not available, secondary data information may be helpful for verification of the cut-off.

Stage 3: Residual Mix (no specific contract with supplier on energy mix or specific data is not available)

When information on supplier-specific electricity is not available or renewable attribute energy certificates have been sold to a third party, a total supplier-specific electricity mix can be used and if that is not available, the residual GHG emission factor should be used (market-based approach). This factor represents the emissions that remain after certificates, contracts, and supplier-specific factors have been claimed and removed from the calculation. Organizations should check databases (see chapter 5.2.6) for residual mixes available for their region of operation. Database values are preferred if they cover a cradle-to-gate scope. Alternatively, organizations operating in Europe can use residual mixes from sources such as AIB [AIB 2021- European Residual Mix] to determine their gate-to-gate emission factors. If this source is used, the upstream emission factors must be calculated based on the composition of the electricity mix using database values for the fuels. If AIB RES mix are used, upstream emissions for electricity should be calculated based on the fuels used. Companies operating in other regions should check if residual mix data is available (e. g. for certain US regions residual mixes are published, cf. [Green-e 2021- Residual Mix Emission Rate].

If no residual mix data is available, then as a last quality option according to the GHG Protocol Scope 2 Guidance [GHG Protocol Scope 2 Standard], national grid mixes can be applied. Organizations should check databases (see chapter 5.2.6) for emission factors covering a cradle-to-gate boundary. If no database values are available, organizations can use IEA data as gate-to-gate emission factors. If that route is chosen it is mandatory to calculate upstream emission factors based on the composition of the grid mix applying database values for the fuels.

Further notes on renewable and low carbon energy

The Renewable Energy Directive [EC-Renewable Energy Directive] defines renewable energy or “green” energy RES-E as: “…energy from renewable non-fossil sources, namely wind, solar, aerothermal, geothermal, thermal, hydrothermal and ocean energy, hydropower, biomass, landfill gas, sewage treatment plant gas and biogases”.

Importantly, double-counting must be avoided. According to ISO 14067 [ISO 14067: 2018], no double-counting occurs:

- Where the process that used the electricity and no other process may claim the generator specific GHG emission factors for that electricity.
- Where the generator-specific electricity production does not influence the GHG emission factors of any other process or organization [ISO 14067: 2018].

The purchase and use of green electricity can be considered in the market-based emission factor provided that the criteria in ISO 14067 Chapter 6.4.9.4.4 are met [ISO 14067: 2018].

If a unit is running with 20% certificates of 100% renewable energy, the total production can be claimed as being renewable by 20%. Alternatively, a mass balance approach can be applied to renewable or decarbonized electricity. In this case, the same principles as the mass balance chain of custody (chapter 5.2.10.5) for biomass can be applied.

Renewable energy purchased for specific products may be applied to those specific products. When applying chain of custody models, it should be noted that there may be misalignment with other LCA standards or standards (e.g.: EPDs).

Offsets shall not be used in the calculation of renewable energy.

The same requirements and provisions for Renewable Electricity are applicable to other Renewable and low Carbon Energy forms, including Renewable or low Carbon Thermal Energy.

Additional notes:

- If processes within the system under study are in small island developing states (SIDS, as defined by the United Nations), the PCF or the cradle-to-gate PCF may additionally be quantified using contractual instruments for such processes, irrespective of grid inter-connectivity.
- Contractual instruments are any type of contract between two parties for the sale and purchase of energy bundled with attributes about the energy generation, or for unbundled attribute claims. Contractual instruments can include energy attribute certificates, renewable energy certificates (RECs), or green energy certificates or other accepted certificates in specific markets.
- Characteristics of a generator should include the registered name of the facility, the name of the owners, the nature of the energy generated, the generation capacity and the renewable energy supplied. Additional characteristics can be added to describe the electricity generation.

5.2.8.2 Raw materials

Raw materials are defined as materials that are purchased and used to produce a product. They can be of primary or secondary origin. Secondary materials include for example recycled material. ISO 14040 [ISO 14040: 2006], see chapter 5.2.8.4). Primary raw materials are often named "virgin" materials.

According to the PACT [PACT Methodology], raw materials can be:

- Extracted directly by the company, e.g. mining activities or agricultural production.
- Sourced by external suppliers.
- Toll manufactured.
- Coming from recycling processes.

Chemical products are often based on raw materials that are derived from oil and its derivates. Raw materials supplied to a machine or processing plant are defined as feedstocks.

The PCF calculation shall consider the full upstream life cycles of raw materials; from raw material acquisition and pre-processing or direct generation from natural resources (e.g. mining) to the factory gate. It shall also include disposal of wastes generated during raw material production.

According to PACT [PACT Methodology], material acquisition refers to the extraction of resources from the environment needed to create a product. Pre-processing refers to the refining of all the acquired natural and biogenic resources so they can be used in a production facility. Transportation to and from the sites of resource extraction, pre-processing facilities and production facilities shall also be included.

Information on purchased raw materials and raw materials used in a chemical reaction

In chemical reactions, raw materials can be purchased or used from different sites or different plants within a site.

Production network ratios of chemical products and consumption mixes of raw materials should be defined as a basis for PCF calculations. The relationships between products from different sources should be documented with a bill of materials (BOM) from a reporting system. Intracompany relations between all involved sites of a company can be integrated in a network of information. Representative averages of the production network ratios (percentage rate) should be generated by solving and eliminating inter-company relations. Consolidated BOM will be used for the calculations. Ratios are available for all raw materials needed in one company based on a Supply-Demand-Balance for each production/site/plant and company information. To build averages of inputs of the same raw material from different sources, a mass weighting approach linked with the PCF of the different raw materials sourced shall be used.

The average calculation can be based on:

- External source (purchased from external supplier):
  - Raw material is procured from an external supplier.
  - All purchased raw material comes with a PCF. PCF information needs to be obtained either by supplier-specific PCF provided with the raw materials or by secondary data for the raw material (see 5.2.5 on requirements for primary and secondary data and 5.2.6 on requirements for emission factors).
  - For various suppliers of a raw material, PCF of raw materials should be averaged by amount of purchased volumes. As an alternative, supplier-specific raw materials may be segregated to specific product lines with documented justification.
- Company source:
  - Product is produced per another BOM at the same company.
  - Inter-company transferred product: product is sourced per a BOM from another internal site or even plant.
- Mixed source:
  - Product is produced in another BOM at the same internal site/plant, and/or product is sourced from another site/plant of the company, and product is procured from an external provider [BASF SE [2021]].

The equation in section 5.2.7 shows a basic equation to calculate GHG emissions (CO_2e) from activity data.

(1) Refer to Waste Framework Directive (2008/98/EC) for further definition requirements of by-products.

Data used for raw materials can be primary or secondary data (see chapter 5.2.5). Further requirements on emission factors can be found in Chapter 5.2.6.

There are no minimum data quality requirements (see chapter 5.2.11) for raw materials currently to accommodate the need for a transition time for capability development in the supply chains. It is desirable for TfS or member companies to implement minimum data quality requirements in the future.

5.2.8.3 Transport

GHG emissions from transportation often have a minor impact on the PCF of a chemical product. However, they shall be considered and checked if important to the PCF by an iterative process (see also cut-off criteria, chapter 5.2.3).

The following transportation activities shall be included in a cradle-to-gate PCF:

- Transportation in the supply chain, for example the transportation of raw materials to the company site, or transportation of a raw material from a tier 2 supplier to a tier 1 supplier (if not already considered).
- The transportation of an intermediate product from one production site to another.
- Transportation within one site of a company e.g., transportation to an internal storage location as part of a company's direct activities should be considered.
- GHG emissions of outbound transportation shall not be included in the cradle-to-gate PCF but calculated and reported separately if requested by customers.

In general, the GHG emissions relating to the entire fuel life cycle (i.e., well-to-wheel)[1] shall be considered in the calculation of emissions from transportation.

Transports can either be carried out directly by the reporting company e.g., in company-owned or leased vehicles, or by external transport service providers. As such, the method used to calculate product-related transport emissions is very much dependent on the availability of information such as fuel consumption, distance covered, mode of transport or load specifics.

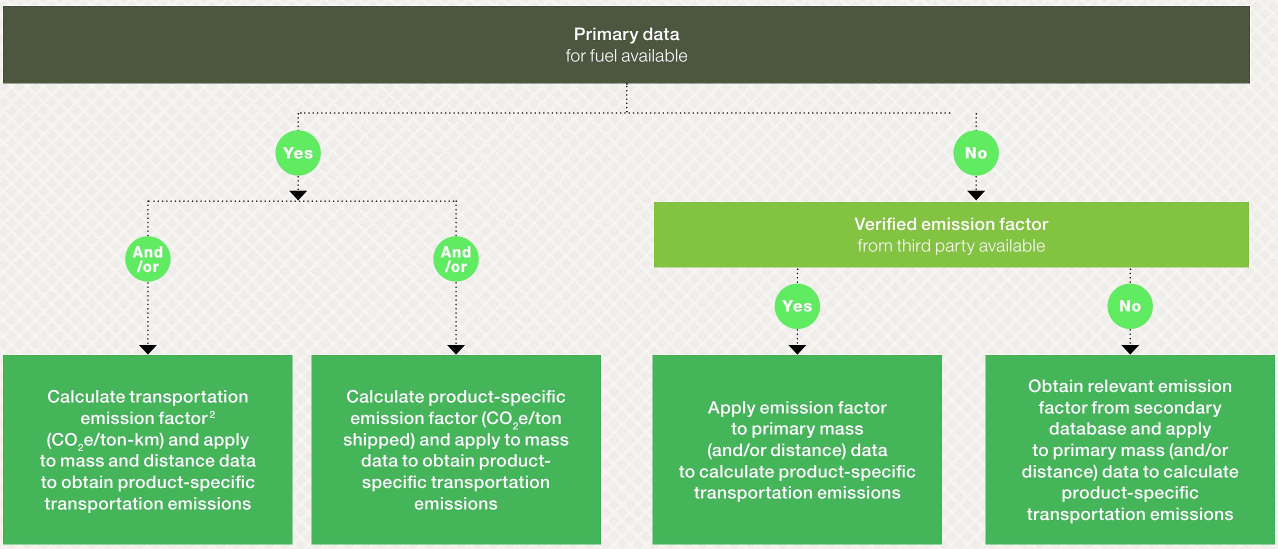
The following paragraphs provide guidance on how to calculate transportation emissions depending on the type of data available (see also Figure 5.6), [PACT Methodology]. This guidance is not available anymore in the updated version of the PACT Methodology formerly known as Pathfinder Framework.

1. If available, primary data on fuel usage should be used to calculate product-related transport emissions, based on actual transportation mode, distance and vehicle load. The fuel consumption data should cover the full round trip that is, include all fuel associated with full, partially loaded, and empty trips, when relevant. Allocation of these emissions shall be based on the mass of the product. In cases where transport is volume limited (full freight's mass is lower than the truck's load capacity) allocation shall be based on volume.

2. Where primary data are not available, but data on product-specific transportation emissions has been shared by the third party operating the transportation, this data should be used and included in the PCF calculation.

3. When a company has neither primary data on fuel usage nor access to product-specific transportation emissions, primary data on mass and most suitable distance shall be used for the calculation of emissions. The relevant emission factor per type of transportation (expressed in CO_2e per tonkm) e.g., provided by the transport service provider, should be applied to this data to calculate product specific emissions. If no emission factor is available, relevant secondary databases shall

Figure 5.6 Calculating product transportation emissions [PACT Methodology]



(1) Well-to-wheel includes the GHG emissions related to fuel production, distribution, and combustions.
(2) Emission factors are always per transportation mode and type.

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be consulted to obtain the necessary emission factor (see section 5.2.6 for suitable databases or [GLEC Framework]).

NOTE: Aircraft GHG emissions have additional climate impacts under certain circumstances at high altitudes because of physical and chemical reactions with the atmosphere. For more information on GHG emissions from aircraft, see the IPCC Guidelines for National Greenhouse Gas Inventories and the IPCC Special Report on Aviation.

Assessment of impacts from transport: example truck transport

Datasets for truck transport are per tkm (ton*km) expressing the environmental impact for 1 ton (t) of product that is transported for 1km in a truck with a certain load. The transport payload (= maximum mass allowed) is indicated in the dataset. For example, a truck of 28-32 t has a payload of 22 t; the LCA dataset for 1 tkm (fully loaded) expresses the environmental impact for 1 t of product that is transported for 1km within a 22 t loaded truck. The transport emissions are allocated based on the transported product's mass and you get only a share of 1/22 of the truck's full emissions. When the load transported is lower than the maximum load capacity (e.g. 10 t), the environmental impact for 1 t of product is affected in two ways. First, the truck has less fuel consumption per total load transported (which is not considered for simplification reasons) and second, its environmental impact is allocated by the load transported (e.g., 1/10 t). When a full freight's mass is lower than the truck's load capacity (e.g. 10 t), the transport of the product may be considered volume limited. In this case, the environmental impact shall be calculated using the real mass loaded. If it is known that empty return transports are the case, the impact of the transportation emission from the round trip shall be considered and attributed to the transported product. For the empty return transport, a reduced emission factor can be considered compared to the full payload.

Based on the assumption of an average load factor of 0.5 net-tons per gross ton can be considered. It can be concluded that the share of empty vehicle-km in long distance transport is still significantly higher for rail compared to road transport. The additional empty vehicle-km for railways can be partly attributed to characteristics of the transported goods.

Therefore, we presume smaller differences for bulk and volume goods and make the following assumptions:

- The full load is achieved for the loaded vehicle-km with bulk goods. Additional empty vehicle-km is estimated in the range of 60% the maximum load for road and 80% of the maximum load for rail transport.
- The weight related load factor for the loaded vehicle-km with volume goods is estimated in the range of 30% of the maximum load for road and rail transport. The empty trip factor is estimated to be 10% for road transport and 20% for rail transport related to the maximum load. These assumptions consider the higher flexibility of road transport as well as the general suitability of the carrier for other goods on the return transport.

EcoTransIT World offers an emission calculator for GHG and exhaust emissions in compliance with EN 16258 and the GLEC Framework [EcoTransIT- Emission Calculator for GHG Emissions].

ISO 14083 was published in 2023 and gives further guidance for transportation. All assumptions and cut-offs considering transportation shall be reported. Furthermore, the Global Logistics Emissions Council (GLEC) developed the GLEC Framework, a globally recognized methodology for harmonized calculation and reporting of the logistics GHG footprint across the multi-modal supply chain may be applied [Global Logistics Emissions Council (GLEC)].

5.2.8.4 Waste treatment and recycling

Manufacturing of chemical products often involves the generation of waste materials, including solids, liquids, gases, and wastewater.

A waste is any material which the holder discards or intends to discard or is legally required to discard per European Waste Framework Directive [EU Waste Framework Directive] or similar national laws. Waste materials that require further treatment before use (i.e. waste for recovery) shall follow the requirements laid down in this chapter. Materials that are identified as waste following the decision tree in Figure 5.7, shall be excluded from the attribution of environmental burdens. Impacts from treatment processes shall be linked to the process, where the waste was generated.

A waste differs from a co-product in that the latter is produced in a multi-output process incidentally to the production of products that are intendedly produced. Figure 5.7 helps the practitioner to decide whether a material can be considered waste or must be classified as a co-product. "Normal industrial practice" can include all steps which a producer would take for a product, such as the material being filtered, washed, or dried; or adding materials necessary for further use; or carrying out quality control. However, treatments usually considered as a recovery operation cannot, in principle, be considered as normal industrial practice in this sense. Some of such processing tasks considered as normal industrial practice can be carried out on the production site of the manufacturer, some on the site of the next user, and some by intermediaries, if they also meet the criterion of being 'produced as an integral part of a production process' (adopted from the EU's Guidance on the interpretation of key provisions of Directive 2008/98/EC on waste).

Co-products as defined in the decision tree Figure 5.7 shall be considered for PCF calculations. See chapter 5.2.9 for guidance on how to account for valuable co-products.

This chapter provides guidance on calculating the burdens and benefits of waste treatment and recycling processes. This is relevant to the PCF calculation in three cases:

- Treatment of wastes generated from operations related to product manufacturing.
- The usage of energy which is recovered from waste incineration for product manufacturing.
- The usage of recycled secondary materials in the manufacturing of the product.
- Preparatory steps and supporting activities for all waste treatment- like collection, transportation, sorting, dismantling, or shredding- shall be considered and included in the PCF calculation following the guideline as described below.

Due to the cradle-to-gate boundary of the PCF calculation within this guideline, emissions from the use and end-of-life stage of the product itself shall not be included in the PCF calculation. If materials are used for the product as raw materials in a circular approach, they shall be considered following the relevant chapters in this guideline. Only the net use of raw materials in the reporting year has to be considered. Any extra impacts used to operate the closed-loop recycling shall be included in the system boundary.

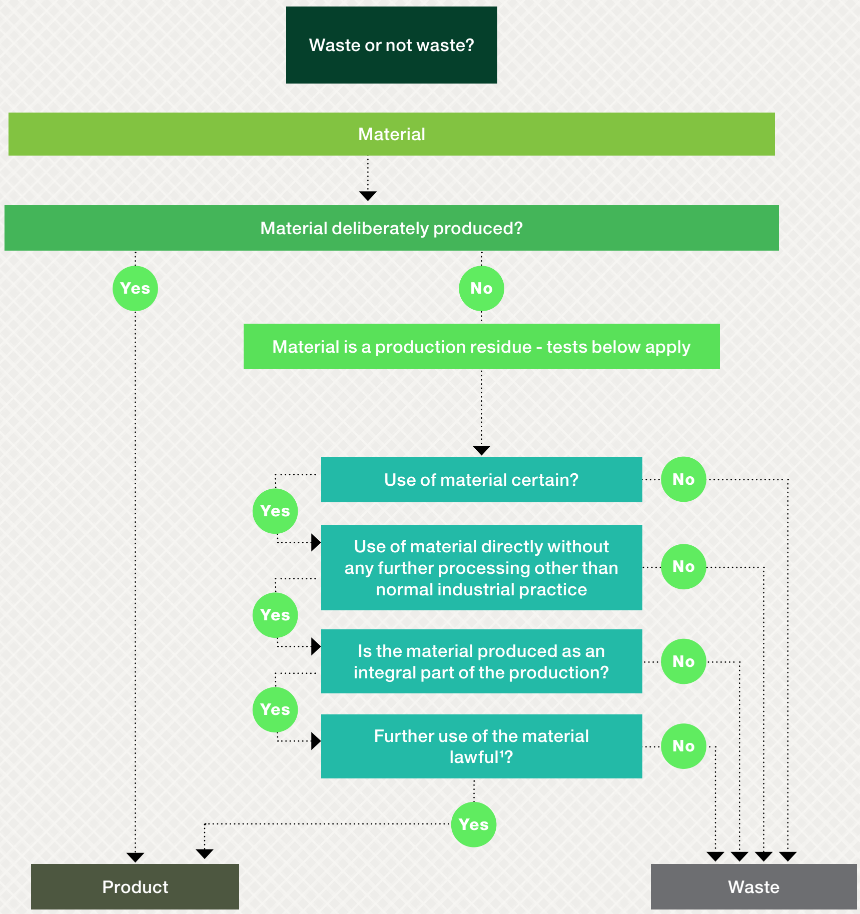
For the consideration of biogenic carbon please refer to chapter 5.2.10.1.

Emission factor sources:

- Whenever possible, companies should use waste treatment emission factors based on primary data.
  - If the waste is treated by the company who generates it, the emission factor shall be calculated based on internal primary data.
  - If the waste is sent to a third party for treatment, the treatment provider shall calculate their waste treatment emissions, develop emission factors, and verify and communicate these to the company who has generated the waste. The emission factors from the third-party treatment shall be calculated based on the TfS approach.

- If primary emission factors cannot be obtained, secondary emission factors shall be used in the following hierarchy:
  - Emission factors shall be estimated based on available information on the waste composition and process technology and parameters of the applied treatment technology. The calculation shall be based on the TfS approach.
  - If this is not possible, emission factors should be derived from accepted secondary databases (chapter 5.2.6).
  - In the case of no data is available, some proposals to develop proxies for landfilling and Wastewater treatment are shown in the appendix.

Figure 5.7 Decision tree from Guidance on the interpretation of key provisions of Directive 2008/98/EC on waste



(1) If the use of materials is lawful needs to be checked specifically for the region, e.g. in Europe Article 5(1)(d) Waste Framework Directive (WFD).

Specifications

Guidance on calculating emission factors for waste treatment and disposal
Emissions from the treatment of non-recycled waste generated during production shall be allocated to the main product or co-products and therefore shall be reflected in the PCF.

Typical waste treatment operations include disposal activities such as:

- Landfill.
- Wastewater treatment.
- Incineration without energy recovery (see example 1).
- Hazardous waste treatment.

In some cases, different types of waste streams are co-treated in a single waste treatment facility, for example in the case of co-incineration of high and low calorific value waste streams or wastewater treatment for wastewater streams with different compositions. Such a waste treatment processes are multifunctional, regardless of whether it includes energy recovery. If data is available, then the impact of the incineration process shall be allocated to the different waste types following the allocation hierarchy for multi-functional processes as described in chapter 5.2.9.

Example 1: Waste incineration without energy recovery

Waste from the manufacturing process of product A is incinerated without energy recovery (either on site or by a third party) as shown in Figure 5.8.

The impact of the incineration process should be calculated or estimated based on the requirements outlined in this guideline. The resulting emission factor shall be allocated to the PCF of product A.

Guidance for calculating emission factors for waste treatment with energy recovery

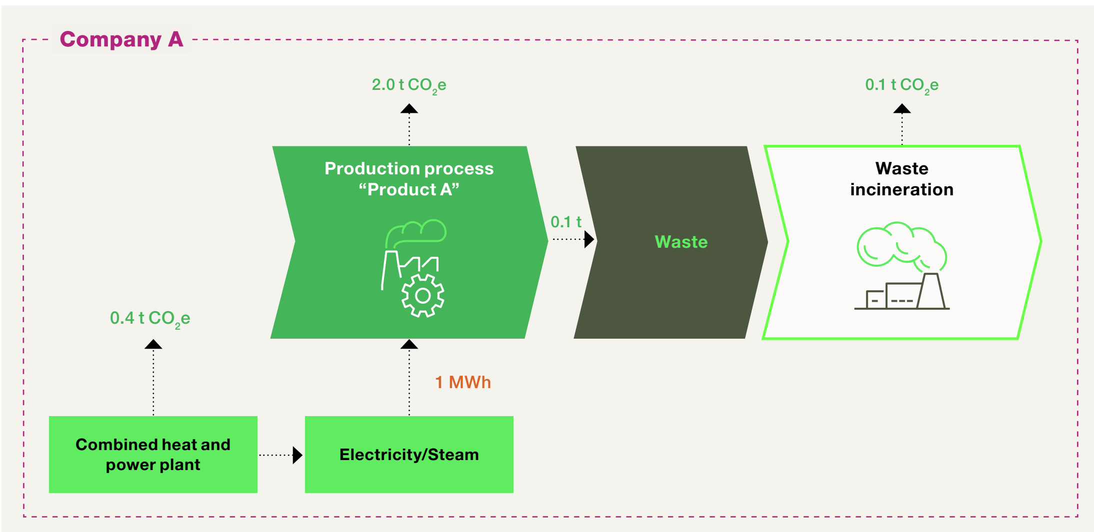
"Energy recovery from waste is the conversion of non-recyclable waste materials into usable energy such as heat or electricity, through a variety of processes, including combustion and other processes to recover energy. This process is often called "waste to energy" [EPA].

The impact of waste treatment with energy recovery shall be included in the product life cycle inventory and system boundary following the calculation approach outlined in this sub-chapter.

Material recycling processes are such processes that derive a secondary material from a waste material which is further used as material for manufacturing of products. Such processes are for example chemical recycling through pyrolization, distillation or mechanical recycling. Guidance on the calculation approach can be found in this chapter under the headline "Guidance for calculating emission factors for material recycling".

Material recycling and waste treatment with energy recovery are considered separate and not equal.
To reduce the emission of GHGs, the chemical industry

Figure 5.8 Waste incineration without energy recovery and without use of the energy



$PCF_{Product\ A} = 2.0\ t\ CO_2e / t + 0.4\ t\ CO_2e / t + 0.1\ t\ CO_2e / t = 2.5\ t\ CO_2e / t$

should strive to keep carbon in a material loop. This is primarily achieved through the reduction of waste generation and material recycling of remaining waste. The impact attribution approach should be designed to incentive both.

Incineration is the least favorable solution because it is a final disposal. The different available calculation approaches regarding waste treatment with energy recovery have been discussed among TfS group members and no consensus has been reached so far. This document in the current state discusses three approaches, which are described with their pros and cons below (Table 5.3). One of the three allocation approaches shall be followed. The choice shall be documented and communicated through the additional information of the PCF.

The discussion to select the most appropriate guidance in this chapter will be continued inviting additional stakeholders to contribute. The guideline will be updated accordingly to reflect changes and consensus. TfS also encourages the development of targeted solutions for such cases through among others, product category rules.

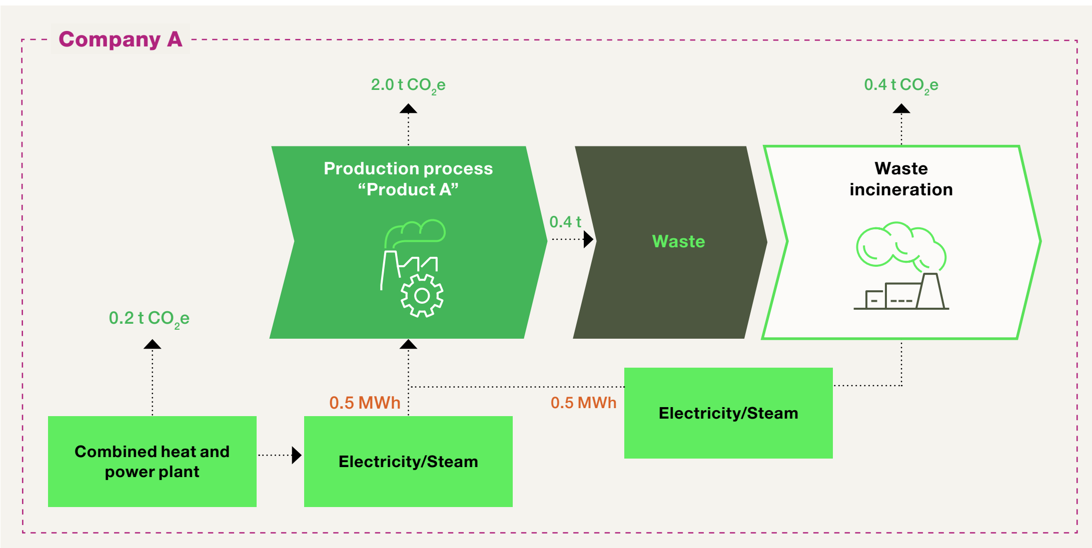
Energy recovery within the system boundaries of a product

If all processes related to energy recovery from waste are included in the system boundary, an allocation is not required, or all allocation approaches lead to the same result. This is the case if the energy generated is directly used in the process of the studied product. The impact of the waste incineration shall be included in the PCF (see Example 2). This closed loop recycling means that the direct recycled energy has no additional environmental impact (= 0). The same applies for material recycling within the system boundaries, as described in the sub-chapter below.

Example 2: Waste incineration with energy recovery within the system boundaries

Waste from the manufacturing process of product A is incinerated with energy recovery on-site and under operational control. The recovered energy is used in the production process of Product A. Since the recovered energy is used within the system boundaries of Product A, no allocation is needed. All CO_2e emissions from the process shall be attributed to Product A as shown in Figure 5.9.

Figure 5.9 Waste incineration with energy recovery within the system boundaries of the company



$PCF_{Product A} = 2.0\ t\ CO_2e/t + 0.2\ t\ CO_2e/t + 0.4\ t\ CO_2e/t = 2.6\ t\ CO_2e/t$

Specifications

Energy recovery outside of the system boundaries of a product

Waste material is part of the life cycle of a product system. It can be treated with energy recovery and this energy can be used in additional product systems. This creates the need to split the impact of the treatment process and identify the part of the impact to be added to each product system.

The following general rules shall apply:

1. Whenever applicable and possible, process subdivision shall be used to divide common processes to avoid the need for allocation [GHG Protocol Product Standard (2011)].
2. For waste treatment with energy recovery, whenever available, allocation methods in line with published and accepted product category rules (PCR) shall be applied.
3. If none of the above apply, either of the three allocation approaches described below shall be applied. The choice shall be documented and communicated through the additional information of the PCF.

The following table describes the three different approaches and discusses its pros and cons. Any of the three methods can be used until further updates following ongoing discussions through TfS.

Table 5.3 Overview of different assessment approaches

	Cut-off approach [GHG Protocol Product Standard, (2011)] also known as recycled content approach	**Reverse Cut-off approach** also known as waste allocation	**Substitution**
Description	"Energy producer takes control" All burden allocated to generated energy	"Polluter pays" All burden allocated to waste generation process	"Market implications considered" Emissions from incineration reduced by credit for substituted energy
Who carries the burden?	Energy user(s)	Waste generator	Energy user(s) and waste generator
Who receives the benefit?	Waste generator	Energy user	Energy user(s) and waste generator
Pros	+ Incentivizes waste treatment with energy recovery compared to without + In alignment with GHG Protocol and PACT Methodology + Simple to apply	+ Incentivizes waste reduction + Incentivizes energy recovery from waste treatment + Simple to apply + Simple data exchange (waste generator provides waste data for calculation and receives emission factor)	+ Incentivizes waste treatment with energy recovery compared to without + GHG & ISO conform + Commonly implemented in LCA databases + Incentivizes waste reduction if more renewable energy is available
Cons	– No incentive for material recycling compared to energy recovery – No incentive to reduce waste – No incentive to use energy compared to renewable energy (Higher emission factors compared to best technology) – Some LCA database need to be adjusted	– Deviates from GHG Protocol – No difference in energy emission factor compared to renewable sources – Lower incentive for energy reduction – Some LCA database need to be adjusted	– Result depends strongly on selected comparative system for substitution – Complex data exchange data for comparative solution required (market data) and agreed by energy user and waste provider
Link to/ Implications for corporate GHG emissions reporting	In line with corporate Scope 3 GHG reporting	Not in line with corporate Scope 3 GHG reporting	Substituted emissions need to be reported separately

Following the cut-off approach (also known as recycled content approach):

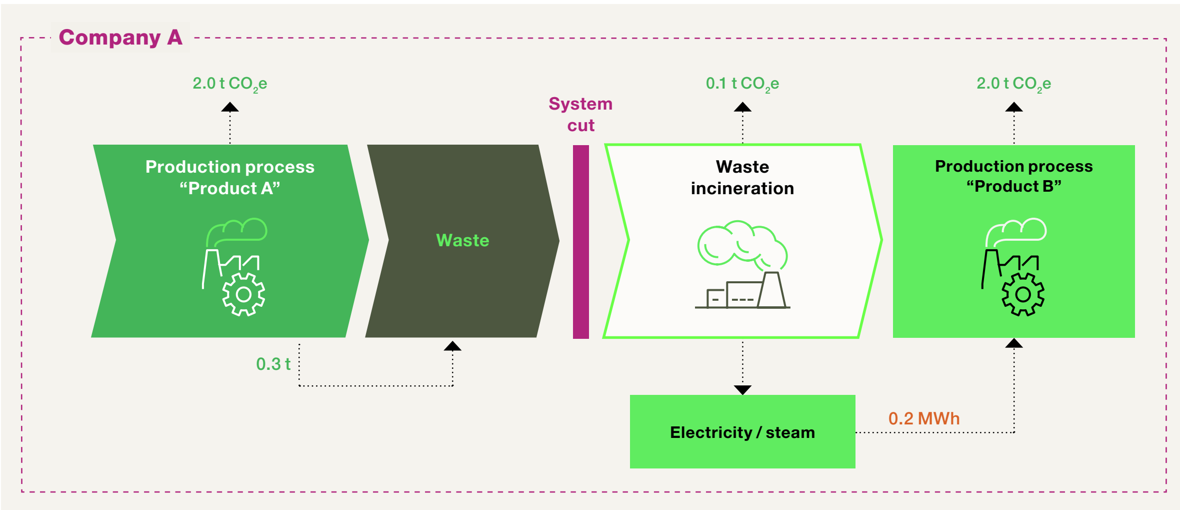
- The impact of preparatory steps and supporting activities such as collection, transportation, sorting, dismantling, or shredding shall be added to the inventory results of the product system producing the secondary product.
- The waste input to the energy recovery process shall be treated as free of burdens. Burdens or credits associated with material from previous or subsequent life cycles are not considered i.e., are "cut-off".
- The impact of the energy recovery process shall be added to the inventory results of the product that uses the energy.

Example 3: Energy recovery with several product systems (cut-off approach)

Organic solvent waste from the manufacturing process of the product A is treated in a waste incineration process with energy recovery on-site and under operational control. The recovered energy is not used in the manufacturing process of product A. It is used in the manufacturing of product B.

Following the cut-off approach, the impact of the waste treatment process shall be allocated to the user of the energy, product B. No impact from the production process for product A shall be allocated to the PCF of product B. If any of the processes, e.g. the production process "Product B" is not operated by company A but operated by a third party, the same approach shall be applied.

Figure 5.10 Energy recovery from waste incineration with application of the cut-off approach



$PCF_{Product A} = 2.0\ t\ CO_2e/t$

$PCF_{Product B} = 2.0\ t\ CO_2e/t + 0.1\ t\ CO_2e/t = 2.1\ t\ CO_2e/t$

$PCF_{Energy} = 0.1\ t\ CO_2e/0.2\ MWh = 0.5\ t\ CO_2e/MWh$

Following the reverse cut-off approach (waste allocation approach)

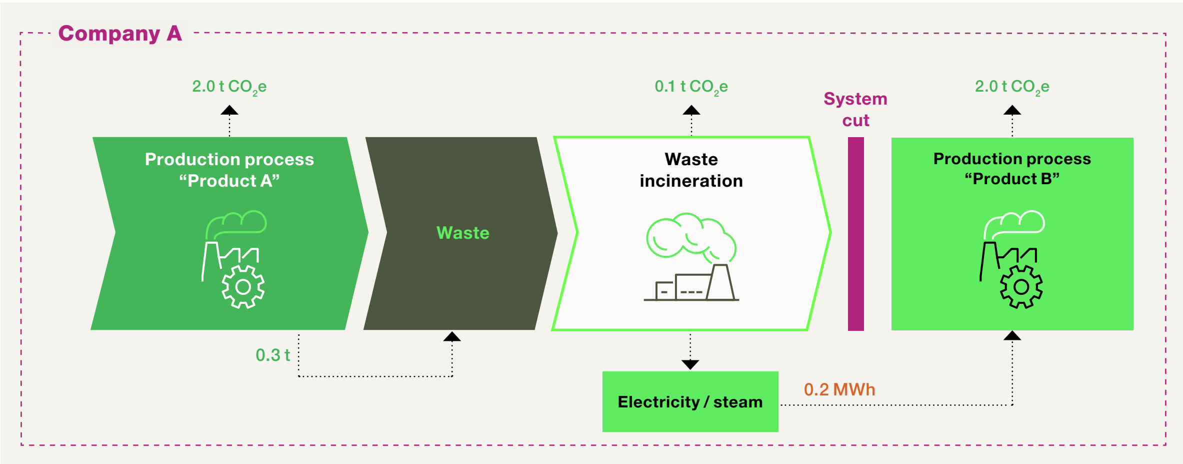
- The impact of preparatory steps and supporting activities such as collection, transportation, sorting, dismantling, or shredding shall be added to the inventory results of the product system generating the waste.
- The impact of the process treating waste with energy recovery (e.g. incineration) shall be added to the inventory results of the product system that generated the waste treated in the process.
- The energy recovered from the waste-to-energy process shall be treated as free of burdens. Burdens or credits associated with previous or subsequent life cycles are not considered i.e., are "cut-off".
- Burden free energy from waste shall be considered when energy recovery is done by the same company (Figure 5.10) since the company generating energy from waste shall report direct emissions.
- Reverse cut-off shall not be applied to material recycling processes which is outlined in chapter 5.2.8.4.
- Reverse cut-off described here is only applicable to product carbon footprint accounting, thus, not applicable to corporate Scope 3 accounting of waste (Scope 3.5) or end-of-life of products (Scope 3.12) with energy recovery.

Example 4: Energy recovery with several product systems (reverse cut-off approach)

Organic solvent waste from the manufacturing process of the product A is processed by a third party in an energy recovery process. The recovered energy is not used in the manufacturing process of product A. It is used in the manufacturing of product B.

Following the reverse cut-off approach, the impact of the waste incineration process shall be allocated to the generator of the waste, product A. The energy shall be considered free of burden, see Figure 5.11.

Figure 5.11 Energy recovery from waste incineration with application of the reverse cut-off approach



PCF $_{\text{Product A}}$ = 2.0 t CO_2e/ t + 0.1 t CO_2e/ t = 2.1 t CO_2e/ t
PCF $_{\text{Product B}}$ = 2.0 t CO_2e/ t
PCF $_{\text{Energy}}$ = 0 t CO_2e/MWh

Following the substitution approach:

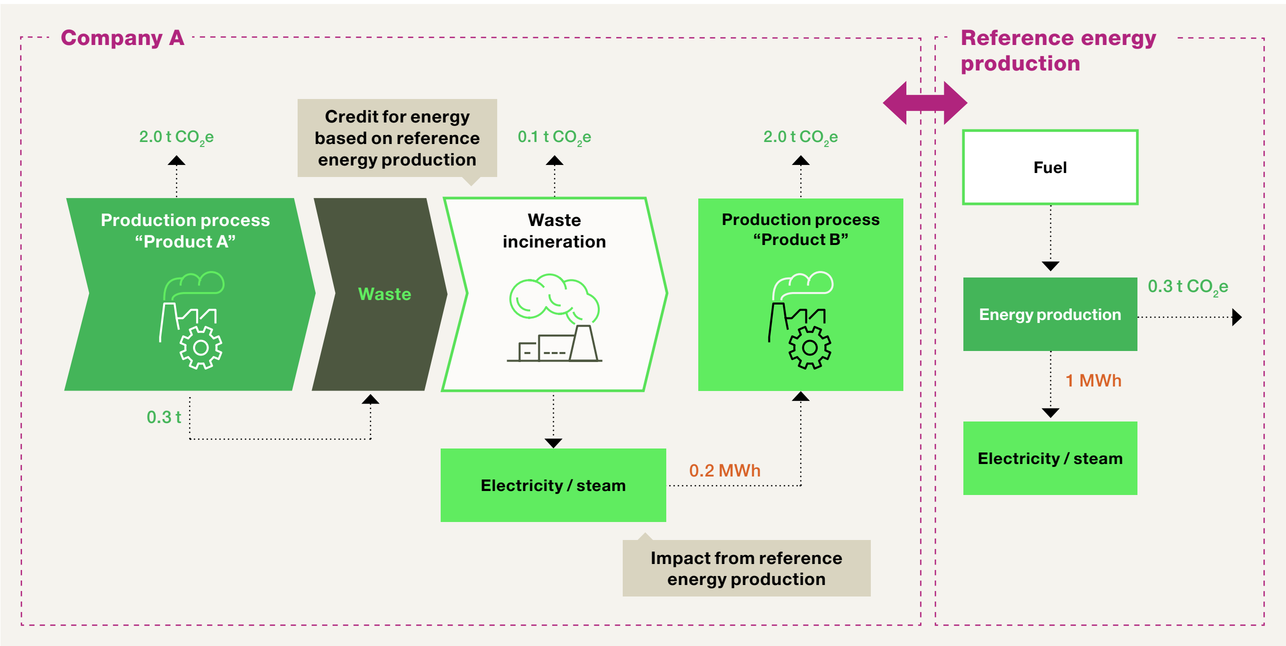
The substitution approach is a method to distribute the impacts of multifunctional process (e.g. waste treatment with energy recovery) between the waste generating and energy using system. Following the substitution approach this is achieved, with the help of including a reference system for energy production. Following this approach:

- The impact of preparatory steps and supporting activities such as collection, transportation, sorting, dismantling, or shredding shall be added to the inventory results of the product system generating the waste.
- The energy recovered from the recovery process (e.g. incineration) shall get a PCF representing the impact of the reference energy production (e.g. steam from natural gas of a combined heat and power plant). This impact shall be added to the product system using the energy. The product system using the energy receives no benefit from waste treatment with energy recovery.
- The impact of the recovery process (e.g. incineration) shall be added to the waste generating systems. A credit shall be subtracted for the amount of energy recovered using the impact of the reference energy production.
- The list of materials that can be a substitute in the substitution approach was created and will be frequently updated. Experiences and requests to be implemented into the list can be sent to TfS for consideration. The list as other information on substitution of materials in defined processes can be found here: **https://www.tfs-initiative.com/pcf-guideline#multioutputprocessesand acceptedpcrs**.

Example 5: Energy recovery with several product systems (substitution approach)

The production process of product A generates a waste (e.g. solvent waste). This waste is incinerated with energy recovery. The energy is used in the production of product B. As reference, energy can be produced by incineration of a primary fuel as shown in Figure 5.12.

Figure 5.12 Energy recovery from waste incineration with application of the substitution approach



$PCF_{Product\ A} = 2.0\ t\ CO_2e/t + 0.1\ t\ CO_2e/t - 0.2\ MWh * 0.3\ t\ CO_2e/MWh = 2.04\ t\ CO_2e/t$
$PCF_{Product\ B} = 2.0\ t\ CO_2e/t + 0.2\ MWh * 0.3\ t\ CO_2e/MWh = 2.06\ t\ CO_2e/t$
$PCF_{Reference\ Energy} = 0.3\ t\ CO_2e/1\ MWh$

Example 6: Energy recovery in a heat network (comparison of the three approaches)

For a comparison of the different approaches, this example is calculated for all three approaches discussed in this chapter. The example shows a simplified scheme of a possible production network in a value chain. The different PCF values for steam and the products calculated with the different approaches are shown in Table 5.5.

Company A produces product A. Waste that is generated in the production of product A is incinerated with energy recovery. In addition to steam generated by the waste incineration with energy recovery, the steam grid consists of a combined heat and power plant and a municipal waste incineration that incinerates product C at its end-of-life with energy recovery.

Both company A and B are using steam in the production of their products. 1 t of product A and 1 t of Product B are produced in the system. 1 t of product C is treated as waste at its end-of-life as shown in Figure 5.13.

Figure 5.13 Example of interlinked system with energy recovery from both production and municipal waste

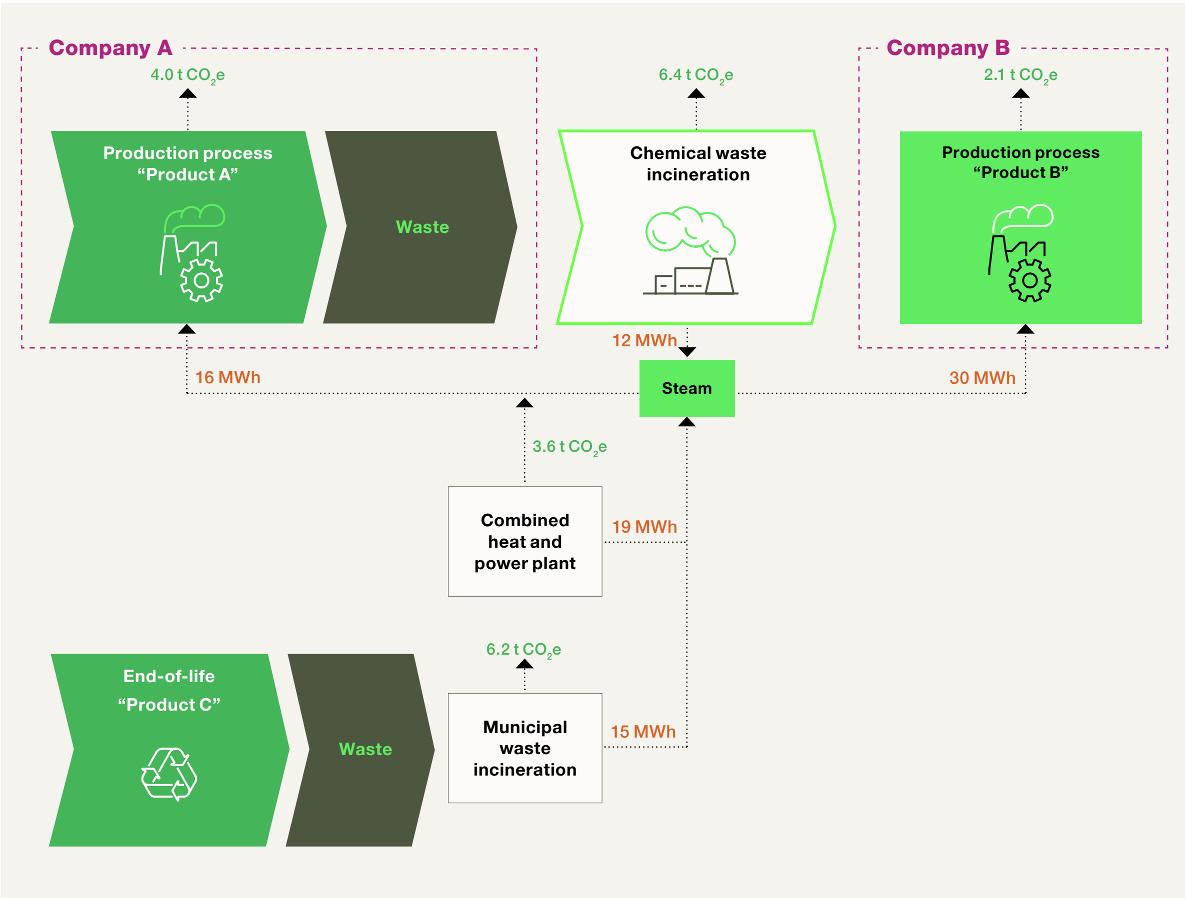


Table 5.4 PCF calculation for example of Figure 5.13 for the different assessment approaches

Unit: t CO_2e/kg (materials) t CO_2e/MWh (steam)		Cut-off approach	Reverse cut-off approach	Substitution approach
Steam	PCF (Steam, combined heat and power plant)	3.6 / 19 = 0.19	3.6 / 19 = 0.19	3.6 / 19 = 0.19
	PCF (Steam, chemical waste incineration)	6.4 / 12 = 0.53	0	0.19 = PCF (Steam, combined heat and power plant)
	PCF (Steam, municipal waste incineration)	6.2 / 15 = 0.41	0	0.19 = PCF (Steam, combined heat and power plant)
	PCF (Steam, total)	(3.6 + 6.2 + 6.4) / (19 + 15 + 12) = **0.35**	3.6 / (19 + 15 + 12) = **0.078**	**0.19** = PCF (Steam, combined heat and power plant)
Product A	Direct process emissions	4.0	4.0	4.0
	Waste incineration emissions	0	6.40	6.40
	Steam emissions	16 * 0.35 = 5.63	16 * 0.078 = 1.25	16 * 0.19 = 3.04
	Steam credit	0	0	12 * 0.19 = 2.28
	PCF (Product A)	**9.63**	**11.65**	**11.16**
Product B	Direct process emissions	2.10	2.10	2.10
	Waste incineration emissions	0	0	0
	Steam emissions	30 * 0.35 = 10.56	30 * 0.078 = 2.34	30 * 0.19 = 5.70
	PCF (Product B)	**12.66**	**4.44**	**7.80**
Product C	**EoL emissions**	**0**	**6.20**	6.2 – 15 * 0.19 = **3.35**

Guidance for calculating emission factors for material recycling

Material recycling processes are processes that derive a secondary material from a waste material which is further used as material for manufacturing of products. Such processes include chemical recycling through pyrolization, distillation of materials or mechanical recycling. The impact of material recycling shall be included in the product life cycle inventory and system boundary following the calculation approach outlined in this sub-chapter.

Recycling within the system boundaries of a product

If all processes related to recycling from waste are included in the system boundary, no specific considerations are required. The impact of the recycling process shall be included in the PCF. This approach is described for waste treatment with energy recovery in example 2.

Recycling outside the system boundaries of a product

Industrial materials can also be recycled along a value chain. Waste material is part of the life cycle of a product system and is reused or recycled as a secondary material in a new product system. This creates the need to split the impact of the processes related to recycling, as they may be shared between two different product life cycles.

To reduce the emission of GHGs, the chemical industry should strive to keep carbon in a material loop. This is primarily achieved through the reduction of waste generation and material recycling of remaining waste. The impact allocation approach should be designed to incentive both.

The different available calculation approaches have been discussed among TfS group members and no consensus has been reached so far. The discussion to select the most appropriate guidance in this chapter will be continued, inviting additional stakeholders to contribute. The guideline will be updated accordingly in due time to reflect changes and consensus. TfS also encourages the development of targeted solutions for such cases through among others, product category rules.

Standards for Product LCAs and corporate sustainability reporting are currently not harmonized and do not fully address the steering effect of PCFs for important technologies with the potential to defossilize the chemical industry, such as chemical recycling. The following methodologies are a proposal by the chemical industry to steer those technologies but are not yet harmonized with the GHG Protocol and other existing standards.

The following section is focuses on the assessment of post-consumer waste recycling. Post-industrial waste streams of high quality and/or high value that will be recycled and used in another application shall be assessment as by-products following the guidance in 5.2.9. This shall not interfere with the waste classification according to legal regulations.

Energy intensive recycling (e.g., chemical recycling) technologies are used to recycle waste streams which cannot be recycled through other methods (e.g. mechanical recycling due to technical and economic reasons). Examples include various types of mixed plastics waste after the sorting step and separating materials that cannot be handled in, for example, mechanical recycling. If a recycling technology enables waste to be used as feedstock (thus preventing less favorable end-of-life options and keeping carbon in the loop), it creates societal benefits in the form of CO_2 reduction and resource savings, and should be acknowledged accordingly.

The following general rules shall apply:

1. Whenever applicable and possible, process subdivision shall be used to divide common processes to avoid the need for allocation. [GHG Protocol Product Life Cycle accounting standard].

2. For secondary material derived from a recycling process, whenever available, "allocation methods in line with published and accepted product category rules (PCR) of analogous processes shall be applied, e.g., Plastics Europe or the [PACT Methodology].

3. If none of the above apply, the two calculation approaches described below shall be consulted.

The first choice shall be a cut off approach due to the requirements of the GHG Protocol [[GHG Protocol Product Standard] with additional requirements on reporting. When providing a cradle-to-gate PCF, the figure for end-of-life emissions shall be reported additionally.

For specified cases, an upstream system expansion approach can be used as an alternative option. In this approach, the cradle-to-gate PCF is provided considering a credit for the avoided waste treatment from the first life cycle.

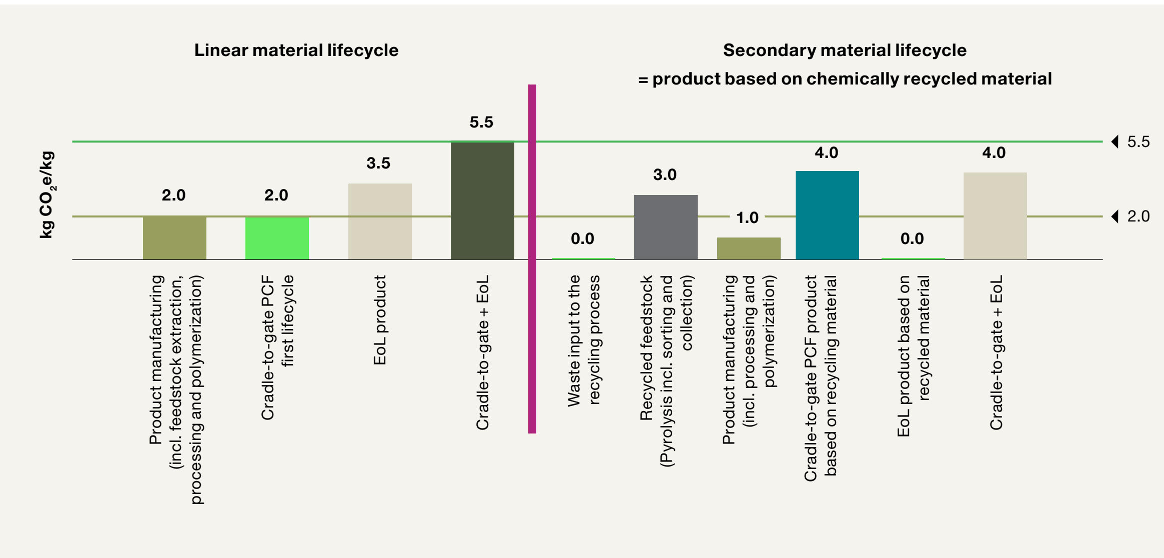
The following text explains both methods and provides examples.

Following the cut-off approach (also known as recycled content approach):

- The impact of preparatory steps and supporting activities such as collection, transportation, sorting, dismantling, or shredding shall be added to the inventory results of the product system producing the secondary product.
- The waste input to the recycling process shall be treated as free of burdens. Burdens or credits associated with material from previous or subsequent life cycles are not considered, i.e., they are "cut-off".
- The impact of the recycling process shall be added to the inventory results of the product that uses the secondary material.
- For the product in scope the PCF of all burden shall be reported. Additionally, the EoL of the virgin alternative should be shown in comparison to the recycled product. This is a specific PCF covering EoL effects as well. With this approach, benefits of the recycling of materials can be shown but are beyond a cradle-to-gate scope.

Details of this calculation approach are shown in example 3 of this chapter.

Figure 5.14 Cut-off and additional information approach - exemplary data



Example Cut-off and additional information

The recycled content method or cut-off in the GHG Protocol for Products allocates the recycling process emissions and removals to the life cycle that uses the recycled material. Furthermore, the recycled content method can be used in open loop situations that include recycled material inputs and outputs.

In this guideline the cradle-to-gate system boundary is in focus hence recycling activities are not visible since they are executed downstream. If recycled materials are used in a process, the benefit are not visible compared to a linear product life cycle. Therefore, the recycled product often has no visible benefit. To show the whole picture, the application of the cut-off calculation can be extended by adding of the end-of life scenario. The “Cut-off plus” approach adds the assumed EoL technology to the cut-off figures linked to the linear material life cycle. Through the additional information provided by the “plus” in “cut-off plus”, the benefit of the recycled material compared to a linear material without the use of recycled input becomes apparent. In Figure 5.14 the single contributions to the PCF are shown.

Standard reporting for cut off as follows:
PCF linear material life cycle (cradle-to-gate first life cycle) = 2.0 kg CO_2e /kg
PCF secondary material (cradle-to-gate second life cycle) = 3.0 kg CO_2e /kg
Additional reporting information: PCF linear material life cycle incl. EoL = 5.5 kg CO_2e /kg
PCF secondary material incl. EoL = 4.0 kg CO_2e /kg

The assumed EoL technology for the virgin material was incineration in Europe based on the C-content of the virgin material. All impact of the incineration was allocated to the EoL including the substitution of the recovered energy. If no further information of the EoL of the virgin material is available, the country mix of disposal technologies of the country of origin shall be considered.

This approach is similar to the cut-off approach described in the GHG Protocol. With the additional information provided by the cut-off plus, the benefit of recycled material compared to virgin material becomes clear.

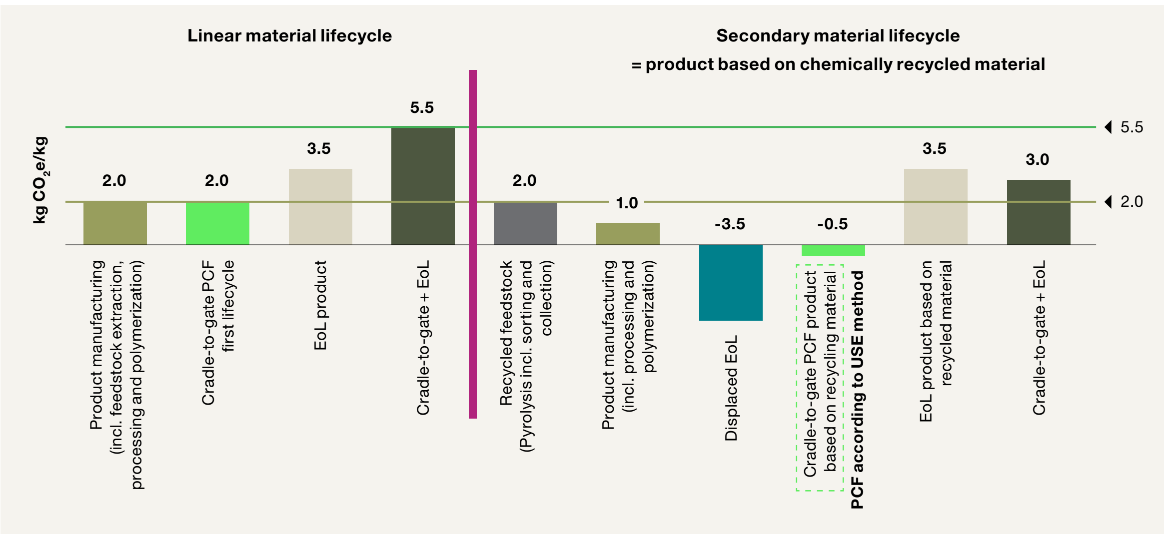
Following the Upstream System Expansion (USE) approach:

In exceptional cases the benefits of a recycled material can be shown using the “Upstream System Expansion (USE)” approach [BASF (2020)]. These exceptional cases shall fulfill all the following criteria:

- Showing a societal benefit in form of overall reduced GHG emissions in comparison to other relevant available treatment methods.
- Being a new technology with a high likelihood of improvement of efficiencies after commercial scale up.
- Ensuring the use of regularly updated data according to the TfS guideline.
- Market for the alternative waste treatments is known with the requirements clearly defined.
- ISO compliant substitution approach is applied and the exact use of the waste is known.
- Substitution shall only be applied if the alternative treatment directly replaces the final disposal, and the process is therefore reduced through provision of the co-product.
- Data about the impact of the alternative production process needs to be obtained to calculate the PCF of the alternative product and compare it to the system under study.
- A clear description of the process for selecting the final EoL option substituted by chemical recycling shall be documented.

The burdens from collection, sorting, recycling step (e.g., pyrolysis) and further processing of the final product (e.g., cracking) are accounted to the secondary material as well the burden of the recycling process. All burdens shall be reported. Additionally, the credit of the displaced EoL impact can be deduced and reported. As a basis for EoL impact estimations, the country mix of disposal

Figure 5.15 Example of single contributions to the PCF with the USE approach.
(Note: data shown assumes that the waste and the product are the same material.)



technologies of the country of origin shall be considered if there is no further information of the EoL of the virgin material available.

In a second step, the emission of the counterfactual scenario (what would have happened with the waste if not used for recycling) must be identified. In the case of chemical recycling, the used waste streams are difficult to recycle and would have been incinerated otherwise. The emissions of the counterfactual scenario need to be calculated, e.g., incineration of mixed plastics including energy recovery using commonly available technologies in the defined region [GHG Protocol Product Standard (2011)].

The final PCF of chemically recycled products results from the burdens of recycling, offset by the savings from the counterfactual scenario. This is because the technology contributes to societal CO_2 savings by replacing less favorable waste treatment. options.

With this approach, benefits of the recycling of materials can be shown but are beyond a cradle-to-gate scope.

Example USE

PCF virgin (cradle-to-gate first life cycle) = 2.0 kg CO_2e / kg
PCF secondary (cradle-to-gate based on recycled material)
= -0.5 kg CO_2e /kg

Additional information:
PCF virgin product incl. EoL = 5.5 kg CO_2e /kg
PCF secondary material incl. EoL = 3.0 kg CO_2e /kg

Depending on the methods used, corporate accounting in categories 3.1. and 3.12. may differ and are explained in the description of corporate reporting by TfS.

This approach is different from the existing GHG Protocol approach. The results of the USE method incl. EoL considers a scope beyond cradle-to-gate. To derive a PCF from there can be further addressed in a stakeholder alignment process. The accounting for the EoL along the value chain among the recyclers and users of the material should be a part of this.

5.2.8.5 Direct emissions

Direct emissions are emissions from processes owned or controlled by the company arising from:

- Chemical reactions.
- Waste treatment with and without energy use (e.g., flares).
- Fuel and residues incineration in process plants.

Direct emissions shall be calculated by determining the amount of emitted GHGs based on stoichiometry, mass balance or measured data. The emissions shall then be multiplied with the respective global warming potential (GWP) to calculate the emission factor as CO_2e per declared unit. When relevant, fossil and biogenic direct CO_2e emissions to be reported separately according to the guidance in chapter 5.2.10.1.

5.2.9 Multi-output processes

This chapter is about attributing inputs and emissions 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 with a defined economic value such as a residual fuel. Herein Energy is understood as direct energy e.g., from exothermal reactions [PACT Methodology]. Waste materials that go directly to incineration or landfill, are not co-products and hence, shall be excluded from the attribution of environmental burdens of the multi-output process. The energy generation from waste incineration is described in the waste treatment chapter.

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):

1) The approach described in published and accepted product category rules (PCR), Industry Association projects, directives as e.g. REDII where available, for corresponding product systems shall be applied (see 5.2.4 Standards used). When more than one PCR exists for a product or product category, priority shall be given to allocations rules as described in chapter 5.2.9.3.

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 PCF 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 in 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.

Substitution, as described in chapter 5.2.9.1, may be applied to attribute impact to co-products in multi-output situations if all of the following apply:

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 PCF of the alternative product.

d. There is consensus for a production path of the displaced product agreed by TfS. Note: TfS will maintain and publish a positive list of processes and products.

4) In all other cases companies shall allocate the impact to co-products following the allocation rules described in chapter 5.2.9.3. The applied approach to solve multi-functionality shall always be stated and justified.

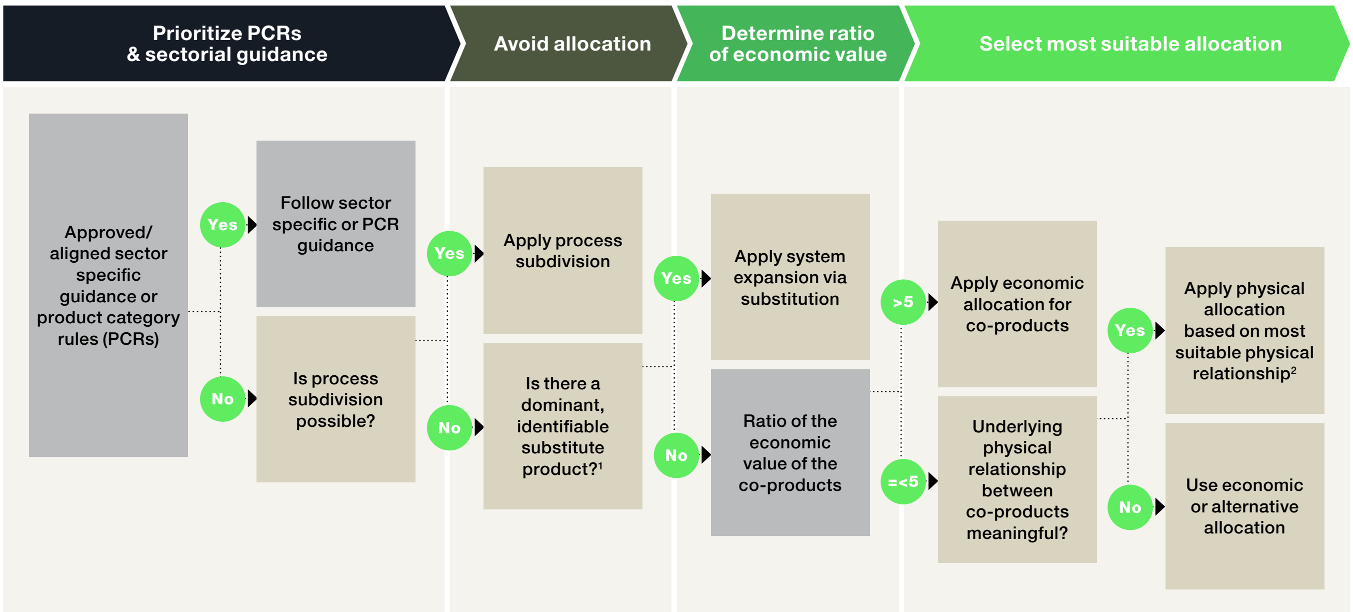
TfS is aligned with PACT Methodology, Catena-X, GBA on the allocation hierarchy and thus the allocation approach as described in a PCR might be prioritized before System expansion and substitution. Since the PCR is ranked very high, it will overrule other approaches.

5.2.9.1 Substitution

In Substitution, the co-products of process are compared to similar alternative products, and the environmental burdens associated with the alternative product(s) are subtracted from the product system under study to obtain the impact of the main product of the production process (see Figure 5.17) [ISO 14044: 2006].

The use of substitution as a means to avoid allocation requires an understanding of the market for the co-products. To ensure that an ISO compliant substitution approach is applied, the exact use of the co-product needs to be known. Substitution shall only be applied if the co-product, which must not be the main product, directly replaces the alternative product on the market and the production of this alternative product is reduced through provision of the co-product. Data about the impact of the alternative production process needs to be obtained to calculate the PCF of the alternative product and subtracted from the system under study. If a co-product and substituted alternative process fulfill all above mentioned requirements, they may be considered for adoption in the TfS positive list. The list of materials that can be a substitute in a multi-output process was created and will be frequently

Figure 5.16 Decision tree to show allocation rules and reduce assessment burden downstream [Harmonized between TfS, Catena-X, PACT, Global Battery alliance]



New elements added to GHG P allocation hierarchy

(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.

updated. Experiences and requests to be implemented into the list can be sent to TfS for consideration. The list can be found here: **https://www.tfs-initiative.com/pcf-guideline#multioutputprocessesandacceptedpcrs.** A clear description of the process for selecting the alternative product substituted by the co-product shall be documented.

Energy co-products such as residual fuels or excess steam shall be treated by substitution if these co-products substitute products that would have been otherwise generated from a primary energy source. Please see further explanation in below example.

5.2.9.2 Examples for Substitution

In the example both co-product A and co-product B are produced as co-products of the same process. The process produces 2 t co-product A and 1 t co-product B with associated CO_2e emissions of 5 t CO_2e (see Figure 5.18).

After application of the decision tree of Figure 5.7, the compound B is identified as an unavoidable co-product. After application of the decision tree of Figure 5.16, it was found that a process subdivision is not possible and a product category rule does not exist. After application of the decision tree of Figure 5.17 it was found that the process is operated and optimized to produce co-product A as the main product. The co-product B is the same product as product B derived from a single output production process and substitutes product B (material or energy) from a single output process.

In the market, co-product B directly substitutes an alternative product B, produced through a process with an impact of 3 t CO_2e/1 t product B. This impact is now assumed for co-product B from the system under study. As the process under study produces 1 t of product B within the system boundaries, the impact of the substituted alternative process can be subtracted from the total impact of the process. As a result, 2 t of co-product A have an impact of (5-3) t CO_2e = 2 t CO_2e. As a result, co-product A has a PCF of 1 t CO_2e/t co-product A.

Figure 5.17 Decision tree for the application of substitution in the co-product assessment

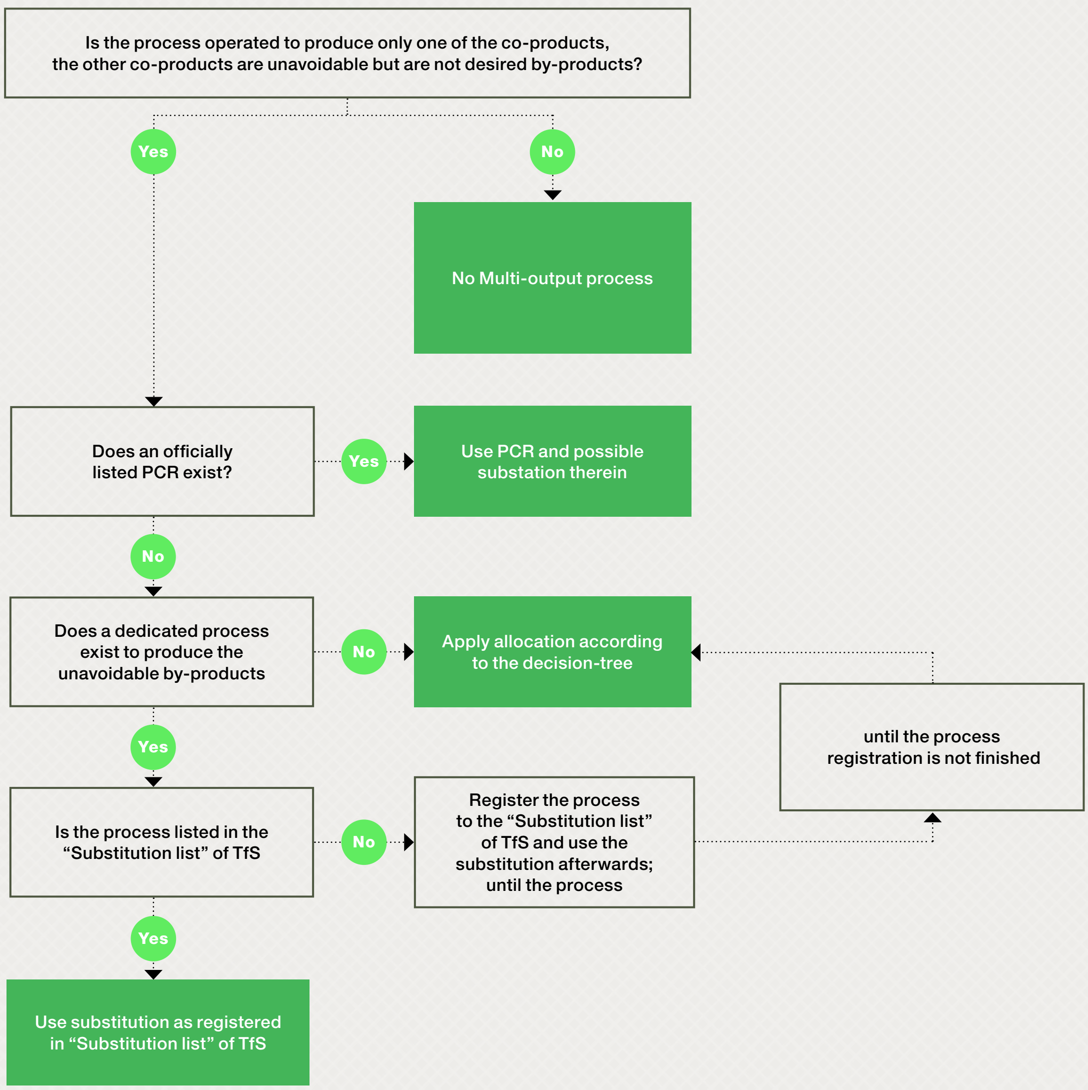
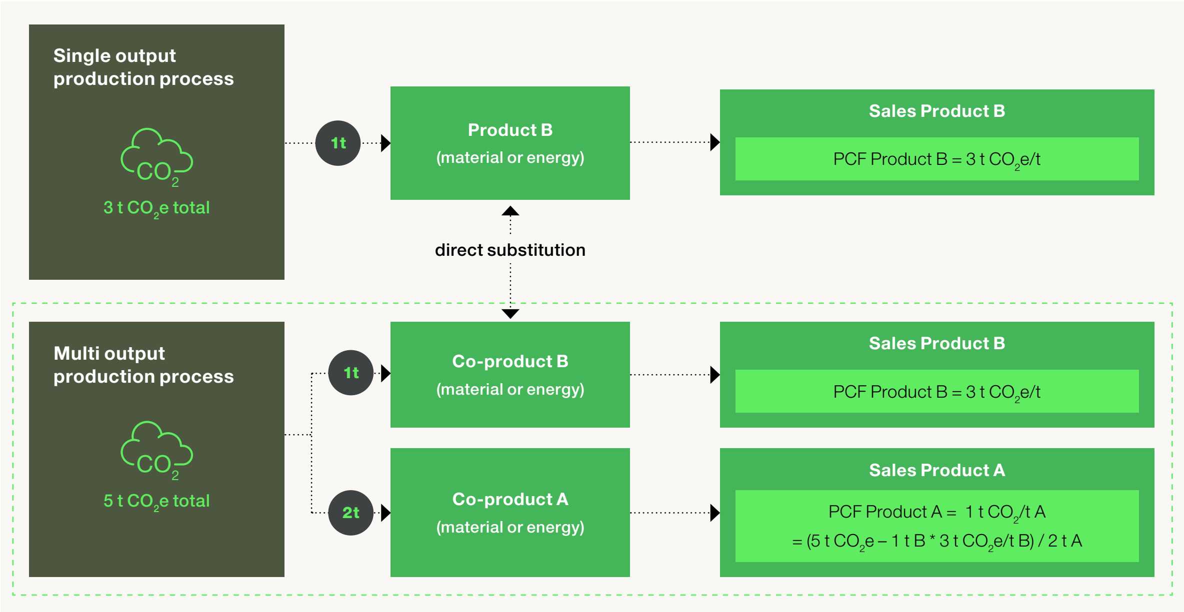


Figure 5.18 Substitution and its modelling of multi output processes



5.2.9.3 Allocation rules

Allocation means splitting multi-output processes into single output unit processes using physical, economic, or other criteria by partitioning the input and output flows of a process or a product system between the product system under study and one or more other product systems. When outputs include both co-products and waste, the inputs and outputs shall be allocated to the co-products only.

There are different allocation methods applicable for the case of a multi-output process. ISO 14067 [ISO 14067: 2018] differentiates between allocation based on the underlying physical relationships between the products and co-products such as mass, volume or energetic content and economic allocation – where physical relationship is the preferred choice. Furthermore, input materials such as chemicals can be allocated by stoichiometry to the products according to the chemical reaction and elemental connectivity.

The following general rules shall apply:

If the multi-output situation cannot be avoided, emissions shall be divided among the co-products in an accurate and consistent manner. This is essential for the quality of a PCF. Allocation rules shall follow the hierarchy described in figure 5.16. [PACT Methodology]:

a) Allocation methods in line with published and accepted product category rules (PCR) of analogous processes shall be applied where available (see 5.2.4 Standards used). In multi-output cases where a PCR applies, the TfS reporting requirements according to the **TfS Data Model** shall overrule any reporting requirements in the PCR. When more than one PCR exists for a product or product category, priority shall be given to allocations rules accepted by TfS in a published list or PCR given in:

1. Existing regional law or regulation.
2. PCRs from worldwide operating associations.
3. PCRs from regionally operating associations. e.g., Plastics Europe).
4. PCR from EPD programs.

b) The guidance of the WBCSD Chemicals [WBCSD Chemicals LCA Guidance (2014)] used the application of the economic value of co-products as a criterion to decide between physical allocation and economic allocation firstly. The criterion for economic allocation was adopted as well by PACT and aligned with TfS (Figure 5.16). Economic allocation factors should be calculated based on stable market prices, as a yearly average or over multiple years in case of high fluctuation (e.g. >100%) of prices to average out high fluctuations of prices, influencing the outcome of an allocation process based on economic values as prices [BASF SE (2021)].

If global or regional market prices are not available, other economic factors as production costs, internal costs, sales prices etc. can be applied.

If the share of a co-product is very small (in mass or volume < = 1%), it can be skipped in the decision about the allocation method (see also Chapter 5.2.3 for rules on cut-off criteria). If there are more than two co-products, use the highest and lowest value of all co-products to determine the value ratio.

Exceptions to the above allocation rules are possible only in rare instances such as:

1. Carbon dioxide that is captured and used as input in another process shall be calculated according to Chapter 5.2.10.4 Carbon Capture and Utilization.

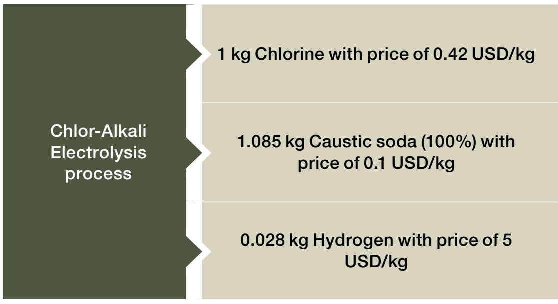
2. If hydrogen is a co-product allocation by heating value shall be applied because of the low molecular weight of hydrogen. Example: Syngas process that generates CO and hydrogen, both are gases and valuable products. If hydrogen is a co-product in a multi-output process, mass allocation shall not be applied because of the low molecular weight of hydrogen.

The applied approach to solve multi-output situations shall always be stated and justified, and the sum of the allocated inputs and outputs of a unit process shall be equal to the inputs and outputs of the unit process before allocation.

5.2.9.4 Examples for allocation

The allocation procedure has a significant impact on the PCF result as can be seen below in the example of Chlor-Alkali Electrolysis, a multi-output process generating chlorine, caustic soda, and hydrogen (see Figure 5.19). Hence a uniform approach for how to deal with multi-output situations for all possible types of product and co-products is needed to generate consistent and comparable results.

Figure 5.19 Outputs of a Chlor-Alkali electrolysis process



It should be noted that an association document exists for Chlor-Alkali Electrolysis and the different allocation approaches shown are simply illustrative examples.

Mass-based allocation

This type of allocation is the distribution according to mass, measured in terms of total mass (see Table 5.5).

Table 5.5 Example calculation for mass-based allocation

Definition	Mass [kg/kg Chlorine]	Share of impact
Chlorine	1.00	47%
Caustic soda (100%)	1.085	51%
Hydrogen	0.028	2%
Sum		**100%**

Stoichiometric or elemental allocation

Stoichiometric ratios of chemical reactions can be used as basis for the allocation. This approach is helpful if mass flows do not reflect the elemental reality of the co-products. This allocation can be used for input materials that have a chemical connectivity only to certain products and not all co-products. Stoichiometric or elemental allocation can be combined with e.g., mass allocation for other raw materials, energy, waste, emissions etc (see Table 5.6).

Table 5.6 Example calculation for stoichiometric or elemental allocation

Definition	Molar mass [g/mol]	Stoichiometric relation to NaCl	Share of NaCl impact
Chlorine, Cl_2	70.9	0.5	60.7%
Caustic soda, NaOH (100%)	40	1	39.3%
Hydrogen, H_2	2	0	0%
Sum			**100%**
Share of NaCl impact = Molar mass of product * stoichiometric factor of product / molar mass of NaCl.			

Economic allocation

The economic allocation refers to the economic value of the products at the location (e.g., in the plant) as well as in the state (e.g., not cleaned) and quantity as provided by the multi-functional process. A specific market price is attributed to each product (see Table 5.7).

If large fluctuations in prices exist, an average price over several years should be calculated to reduce these fluctuations. Most recent prices should be used if available and appropriate.

In cases where the product is not sold or the determination of market prices is hardly possible (e.g. intermediates which are internally used, chlorine for PVC), other approaches might be used, e.g. a combination of production costs and market price of the processed product or the turnover.

Overview of calculation examples with a multi-output-allocation

To support the assessment of materials derived from a multi-output-allocation, the following Table 5.8 gives an overview of established processes and describes how the multi-output-allocation was applied.

Table 5.7 Example calculation for economic allocation

Definition	Value [USD/kg]	Mass [kg/kg Chlorine]	Value x Mass [USD]	Share of impact
Chlorine	0.42	1.0	0.42	60.7%
Caustic soda (100%)	0.10	1.085	0.1085	16%
Hydrogen	5.00	0.028	0.14	21%
Sum			**0.6685**	**100%**

In cases where the product is not sold or the determination of market prices is hardly possible (e.g. intermediates which are internally used, chlorine for PVC), other approaches might be used, e.g. a combination of production costs and market price of the processed product or the turnover.

Table 5.8 General examples for allocation approaches and calculation rules

Example case	Applicable PCF calculation rule "how to do it"
Chlorine-Alkali-Electrolysis delivers besides chlorine, mainly hydrogen and sodium hydroxide; energy co-products such as steam are not generated.	Follow decision tree above: apply allocation scheme as specified in the PCR from [Eurochlor [2022]]. Sodium chloride input is allocated by means of stoichiometry to all products containing either sodium or chlorine atoms (or both): chlorine, sodium hydroxide, sodium hypochlorite and sodium sulphate. Sulphuric acid input is allocated to chlorine production only, since it is used for chlorine drying. Hydrogen emissions are allocated to hydrogen production only, since they refer to losses of hydrogen to the atmosphere. Chlorine gas emissions are allocated to chlorine production only, since they refer to losses of chlorine to the atmosphere. Electricity, steam and all other inputs and outputs are allocated by mass to all valuable products, for solutions to mass content of active molecule.
The steam cracker process turns fossil hydrocarbon feedstocks (predominantly ethane, LPG, naphtha, or gas oil) into several different main products, like ethylene and propylene, benzene, butadiene and hydrogen. The process yields additional further chemicals like, acetylene, butene, toluene and xylene.	This complicated process for a LCA needs some specific approaches for an accurate calculation. Therefore, a PCR from Plastics Europe[1] was developed to harmonize the approach. The PCR distinguishes per definition between so-called "main products" (ethylene, propylene, benzene, butadiene, hydrogen, toluene, Xylene and butenes) and "additional products" (all other products). It is defined that the feedstock used shall be allocated on mass basis to all steam cracker products. Energy demand and emissions shall be exclusively allocated on a mass basis to the "main products" only.
The production of formaldehyde from methanol produces besides formaldehyde excess steam that is used in another production plant at the same site of the reporting company. The steam substitutes steam generated in an on-site CHP plant based on natural gas.	The formaldehyde process produces a co-product which is only used in energy recovery. Following the decision tree and its exceptions, the allocation issue can be solved by system expansion and substitution. This means that the CO_2e impact of the inputs and outputs of the process are completely allocated to the main product. At the same time, however, the process receives a CO_2e credits that corresponds to the CO_2e impact of steam generated in the on-site CHP plant based on natural gas. When using the waste steam as input in another production process it carries the CO_2e burden of the steam generated in the CHP based on natural gas. In this way the CO_2 balance is closed, and the steam generating process is rewarded as it produces a product that substitutes a product that would have been otherwise produced.
Atmospheric gases as nitrogen, oxygen, argon and other inert gases are produced using a process known as air separation. In this process, atmospheric air is split into its primary components via a fractional distillation. Cryogenic air separation units (ASUs) are built to provide nitrogen or oxygen and often co-produce argon. High purity gases can be obtained from this process. Rare gases as neon, krypton, and xenon can be isolated with the distillation of air using at least two distillation columns. This type of distillation can be transferred to almost all other distillations very often used in the chemical industry. The process is applied for the separation of different fractions of chemicals and for the purification of chemicals.	Follow decision tree above: no PCR exists, comparison of economic values of co-products (=prices) results in a ratio of > 5. [Price Product 1 (max) / price Product 2 (min) > 5]. The CO_2e impact from the input and output flows shall be allocated based on an economic allocation approach. If the economic values of co-products (=prices) results in a ratio of =< 5, allocations based on physical relations shall be applied. In a typical distillation process that is applied for the separation of e.g. different chemicals with different boiling points, the boiling points can be used as basis for allocation. Higher boiling points get higher burdens because more energy is needed to distill the products.

(1) Plastics Europe recommendation on Steam Cracker allocation. Plastic Europe- Stream Cracker Allocation

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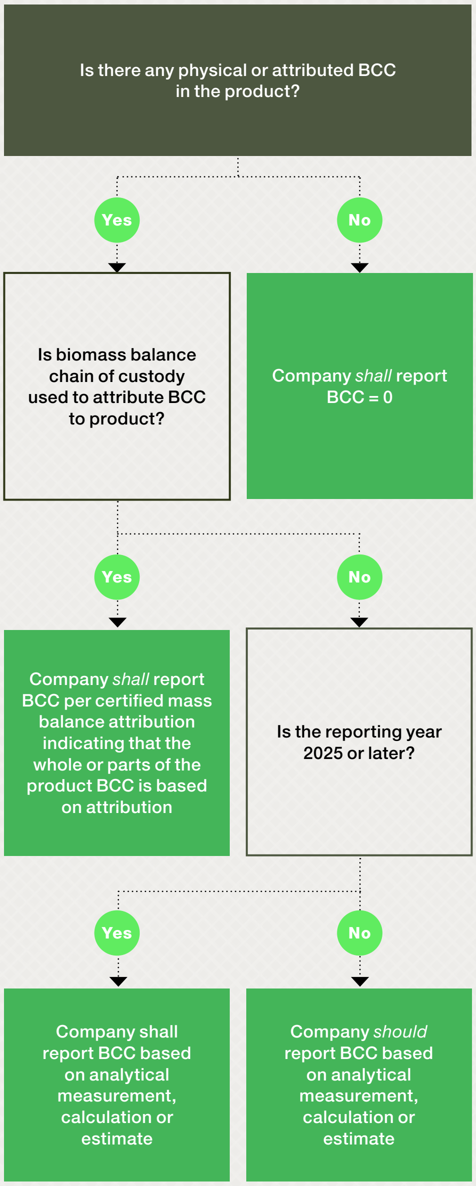
Figure 5.20 Decision Tree for Reporting of Biogenic Carbon Content (BCC) in a Product[1]



Other requirements:

Company shall indicate if BCC is based on physical basis or attribution.

BCC shall be corrected after any economic allocations applied in supply chain.

BCC shall be reported for the products on every life cycle step to allow an accurate modelling of the final product in scope.

(1) 2025 was set as the first mandatory year for reporting biogenic carbon to give all involved companies enough time to prepare for this.

5.2.10 Additional rules and requirements

5.2.10.1 Approach to consider biogenic carbon in the PCF

“During photosynthesis, plants remove carbon (as CO_2) from the atmosphere and store it in plant tissue. Until this carbon is cycled back into the atmosphere, it resides in the carbon pools like bio-based materials. Carbon can remain in some of these pools for long periods of time, sometimes for centuries. An increase in the stock of sequestered carbon stored in these pools represents a net removal of carbon from the atmosphere” [GHG Protocol Corporate Standard]. As bio-based materials originate from plants, the same is true for them and attributed biogenic carbon. If PCF is assessed in a mass balance approach, the biogenic content is attributed. If there is no mass balance applied in the PCF calculation, the biogenic content is physically present in the material and can be measured via C14 analysis. The reported number shows the sum of the attributed and physical BC. Physical and attributed BC is calculated in the PCF as a total of both.

The requirements in this guidance are aligned to the requirements set out in ISO 14067 [ISO 14067: 2018].

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)**.

It should be noted that other systems (namely the European Commission Product Environmental Footprint (PEF 2021) system) treat biogenic emissions and removals differently. PEF does not consider biogenic CO_2 emissions and biogenic CO_2 removals (0/0 approach) so far, but biogenic CH_4 emissions. Furthermore, PEF considers biogenic CO_2 emissions and biogenic CO_2 removals as neutral, independently from its end-of-life treatment. For short term uses of materials with incineration, this approach is identical with the approach of consideration of biogenic carbon uptake and subsequent emission from incineration. To fulfill PEF and current GHG Protocol requirements, additionally the **“PCF (excluding biogenic CO_2 removal)”** shall be reported, which does not consider biogenic removals, but all biogenic and fossil emissions. The biogenic emissions contain the CH_4 emissions that are derived from bio-based C and converted to Methane are transferred to CO_2e. N_2O emissions derived from bio-based materials are expressed in CO_2e as well. If N_2O is emitted from the use of a fertilizer that is based on fossil materials it is linked to the fossil CO_2e.

The upcoming GHG P Land sector and removal Guidance will overrule all the existing GHG P standards in terms of biogenic emissions and accounting requirements. TfS will update this guideline if the final version is published.

Because the prescribed scope of PCF (including biogenic uptake) within this context guideline is a cradle-to-gate consideration exclusively, the total carbon content and the biogenic carbon content of the material shall also be reported alongside the PCF (including biogenic uptake) with the aim to close the biogenic carbon balance in further downstream calculations or at the end-of-life, which are not under the scope of this document [BASF SE (BASF)], [ISO 14067: 2018]. Figure 5.20 presents a decision tree for biogenic carbon content (BCC) reporting. Biogenic carbon is defined as carbon derived from biomass. Biomass refers to material of biological origin and includes both living and dead organic material, such as trees, crops, grasses, tree litter, algae, animals, manure, and waste of biological origin. In this document, peat is excluded from the definition of biomass [ISO 14067: 2018]. Within the context of products, biomass-derived carbon contained in a product is referred to as the biogenic carbon content of the product [ISO 14067: 2018]. BCC may be present in products due to physical presence or due to attribution in biomass balance. If biomass balance is used then provisions shall be in place to avoid double-counting, especially in products which do not receive attributed BCC.

If the mass of biogenic carbon containing materials in the product is less than 5% of the mass of the product, the declaration of biogenic carbon content may be omitted ([EN15804+A2 2019: 46]). The same applies for packaging material if considered and stated in the declared unit.

An example of how to calculate and report the biogenic uptake and the carbon content is presented for a bio-based ethanol below.

- Carbon content in ethanol (number of carbon atoms in ethanol (C=2) x carbon molecular weight (12 g / mol) / total ethanol molecular weight) = (24g/mol / 46g/mol)% = 52.17% C content in ethanol.
- 1 kg ethanol contains 521.7 g C.
- As the biogenic Carbon content accounts 100%, the biogenic C content is also 521.7 g C/kg.
- The biogenic removal is 521.7 g C/kg * 44/12 (conversion of carbon into carbon dioxide) = 1 913 g CO_2 / kg ethanol.

When the ethanol is incinerated e.g. in an EoL process, this amount of CO_2e will be released as emission1. If the ethanol is used as a precursor for a chemical product and this product is applied in a long-term application, the contribution from the ethanol is negative. The new GHG Protocol Land sector and removal Guidance has a new approach on how to account for delayed emissions from product carbon pools. The TfS guideline will be adapted if the Guidance is published.

An example how to report emissions for bio-based ethanol is provided below in Table 5.9.

Table 5.9 Calculation and reporting of PCF results with biogenic materials included

Simplified calculation example: For 1 kg of ethanol	According to ISO 14067: 2018; GHG Protocol Product Standard	According to PEF 2021
Biogenic carbon in products (kg biogenic C/kg ethanol)	0.522	0.522
Equivalent biogenic carbon removal in product, expressed in carbon dioxide (kg CO_2/kg ethanol)	-1.91	0.0
Equivalent biogenic carbon overall removal, expressed in carbon dioxide (kg CO_2/kg ethanol)	-2.31	0.0
Emissions, land use and direct land use change (kg CO_2e/kg ethanol)	0.2	0.2
Of that is direct land use change (kg CO_2e/kg ethanol)		0.1
Emissions, biogenic (kg CO_2e/kg ethanol)	0.4	0.0
Emissions, fossil (kg CO_2e/kg ethanol) (net result of fossil emissions and fossil removals)	2.0	2.0
Cradle-to-gate emission (kg CO_2e per kg ethanol)	-2.31+0.2+0.4+2.0 = **0.29**	0.0+0.2+2.0 = **2.2**

(1) During modeling of EoL, e.g. when biomass is used as energy source for a process, the biogenic carbon in the product should be released in the same way like the fossil carbon depending on the specific EoL technology (e.g. under consideration of conversion into all relevant carbon-based gases (CO_2, CO, CH_4)). It should be checked that the carbon balance is closed (uptake equal emissions).

- *Uptake from biogenic CO_2 emission:*
  0.4 kg CO_2e / kg ethanol
- **Total CO_2 uptake:**
  -1.91 kg CO_2 – 0.4 kg CO_2 = -2.31 kg CO_2

According to ISO 14067 [ISO 14067: 2018] 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.

In some cases, e.g. when allocation is applied, the carbon flows might not represent physical reality in terms of C-content. To avoid misleading or incorrect calculations, a carbon correction shall be applied at the end of the PCF calculations. It must be ensured that the biogenic carbon content in the product is equal to the sum of biogenic removal of CO_2 and biogenic emissions of CO_2 and methane. If this is not the case (e.g. because of allocation somewhere along the value chain) then the value of the biogenic CO_2 removal shall be adjusted.

Consequently, the information shown in Table 5.10 needs to be reported and transferred to the recipient separately (see also Chapter 5.3). In addition, information about carbon content shall be added:

- Biogenic carbon content: 0.522 kg C / kg Ethanol.
- Total carbon content: 0.522 kg C / kg Ethanol
  (= biogenic carbon content of 0.522 kg C / kg product
  + fossil carbon content of 0 kg C / kg product).

For the raw material calculation in section 5.2.8.2 the total figures according to ISO 14067 [ISO 14067: 2018] shall be used. The results for a product calculation includes the biogenic removal at the gate. The biogenic carbon uptake shall be reported in addition. This will enable the calculation of a correct PCF depending on the end-of-life treatment of the final user of the product.

When considering biogenic carbon removal in products for a specified duration, the effect of the timing of GHG emissions and removals shall be assessed [ISO 14067: 2018].

Where GHG emissions and removals arising from the use stage and/or from the end-of-life stage occur over more than 10 years (if not otherwise specified in the relevant PCR) after the product has been brought into use, the timing of GHG emissions and removals relative to the year of production of the product shall be specified in the life cycle inventory. The effect of timing of the GHG emissions and removals from the product system (as CO_2e), if calculated, shall be documented separately in the inventory [ISO 14067: 2018].

The biogenic carbon content of the packaging (if considered in the PCF) shall be excluded or reported separately for an accurate end-of-life calculation.

Biomass used for chemical production should be of high quality and should be produced addressing important sustainability aspects of a high level of sustainability.

Table 5.10 dLUC and iLUC [ISO 14067: 2018]

Direct land use change (dLUC)	Indirect land use change (iLUC); optional
Change in the human use of land within the relevant boundary which leads to a change in soil and biomass carbon stocks. E.g. Primary forest is converted to agricultural land or grassland. GHG emissions and removals associated with these changes from reference land use to land use under assessment need to be addressed and shall be included in the PCF calculation.	Change in the use of land, which is a consequence of direct land use change, but which occurs outside the relevant boundary. E.g. Change in use of agricultural land for food to agricultural land for bio-based chemical feedstocks which lead to shift of food production outside the boundary.

Table 5.11 Examples for avoided emissions by off-setting

Example case	Applicable PCF calculation rule	Voluntary additional information for emission offset
The company purchases emission credits from a project investing in reforestation to offset 50% of the calculated PCF	The PCF remains the same as calculated	The emissions offset of 50% may be provided separately from inventory results
The company purchases emission credits from a carbon capture and storage facility from another company to offset 30% of the calculated PCF	The PCF remains the same as calculated. The GHG reduction by CCS cannot be considered as emission reduction in the PCF, as the CCS is not part of the product system	The emissions offset of 30% may be provided separately from the inventory results

5.2.10.2 Land-use-change emissions

Land use change (LUC) refers to a change from one land use (can be natural habitats such as primary forests or also agricultural land) to another land use (most times to "human use or management of land."). As a result of land use change, GHG emissions and removals occur through changes in soil and above and below ground biomass carbon stocks that are not the result of changes to management of land [ISO 14067: 2018]. Changes in management of land within the same land-use category are not considered land use change (e.g. agricultural land to agricultural land). Land use change can be classified as direct or indirect land use change (Table 5.10):

In accordance with ISO 14067 [ISO 14067: 2018] GHG emissions and removals occurring because of dLUC shall be included in the PCF calculation and shall be declared separately in the documentation [ISO 14067: 2018]. GHG emissions and removals as a result iLUC can be considered for inclusion and – if calculated - shall be documented separately [ISO 14067: 2018].

The **GHG emissions and removals** occurring because of dLUC within the **last decades** (IPCC tier 1 period of 20 years is frequently used) shall be assessed in accordance with internationally recognized methods, such as **the IPCC Guidelines for National Greenhouse Gas Inventories** [IPCC- GHG Inventories Guidelines].

If a specific approach (e.g. based on site, regional or national data) is used, the data shall be based on a verified study, a peer reviewed study or similar **scientific evidence** and shall be documented in the PCF study report [ISO 14067: 2018].

If a product is 100% fossil based including all relevant precursors, this category is of very low relevance and can be neglected in the evaluation and should be reported as "not applicable".

Once the GHG Protocol Land Sector and Removals Guidance is published, a method shall be introduced that allows for insetting CO_2 sequestration in the soil via cultivation of plants (used as raw materials). This method must be able to consider reversals of the sequestrated CO_2 at a later point.

5.2.10.3 Avoided emissions and offsets

Definition of avoided emissions

In this standard, avoided emissions are quantified as emissions reductions that are indirectly caused by the studied product or process or by market responses to the studied product or process that occurs in the studied product's life cycle. Avoided emissions shall not be subtracted from the total inventory results of the PCF.

For more information on avoided emissions see WRI Guideline on avoided emissions [Estimating and Reporting the Comparative Emissions Impacts of Products],
[GHG Protocol Product Standard], [ICCA - Avoided Emission Challenge [2017]] or [WBCSD - SOS 1.5], released 2023.

Definition of emission offsets

"Emission offsets are emission credits (in the form of emission trading or funding of emission reduction projects) that a company purchases to offset the impact of the studied product's emissions. Companies typically use offsets for one of two reasons: to meet a reduction goal that they cannot reach with reductions alone, or to claim a product as carbon neutral" [GHG Protocol Product Standard].

Emission offsets shall not be subtracted from the total inventory results of the PCF. However, if a company wishes to purchase offsets for its product inventory, it may provide information on the offsets separately from the inventory results. For these offsets to be provided separately as additional information, the company should: Purchase offsets for which GHG emission benefits are quantified following internationally accepted GHG mitigation project accounting methodologies (e.g. GHG Protocol Project Protocol); only account for product-level offsets to avoid double-counting of corporate-level offsets [GHG Protocol Product Standard]. Table 5.11 shows examples of off-setting processes.

Definition of emission 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.

Since there are developments towards new ISO standards, aspects might be addressed differently. On ISO Level there is a new standard, ISO 14068-1 "Carbon neutrality" was published in the year 2023. A Net Zero approach of ISO started as well with the International Workshop Agreement IWA 42 Net Zero Guidiong principles. These activities might initiate new calculation aspects and implementation of PCF in specific calculations. This guideline will include elements of these documents if they are further established, accepted in industry and new requirements are needed to be addressed.

5.2.10.4 Carbon Capture and Storage or Utilization

"Carbon Capture" refers to processes where CO_2 is separated from industrial and energy-related sources or technically captured from the atmosphere. This guidance refers only to the capturing of CO_2 at the source of emissions. Direct air capture technologies are out of the scope of this sub-chapter. For other technologies that capture different carbon sources (e.g., CH_4), further definitions are needed.

CCS (Carbon Capture and Storage, or more accurately, CO_2 Capture and Storage) refers to the separation of CO_2 and its injection into a geological formation, resulting in long-term isolation from the atmosphere.

"Long-term" means the minimum period necessary to be considered an effective and environmentally safe climate change mitigation option [ISO 27917:2017], [ISO Guide 84:2020].

CCU (Carbon Capture and Utilization, or more accurately, CO_2 Capture and Utilization) refers to technical processes where the separated CO_2 is converted into valuable products. In contrast to CCS, the CO_2 storage in CCU is only temporary. Emissions can be delayed and thus do not contribute to climate change during the time of storage [Müller, Kätelhön et al (2020)].

CC only refers to industrial emission sources, while biological processes, where CO_2 is also stored (or sequestered), such as planting trees, are not covered by the terminology.

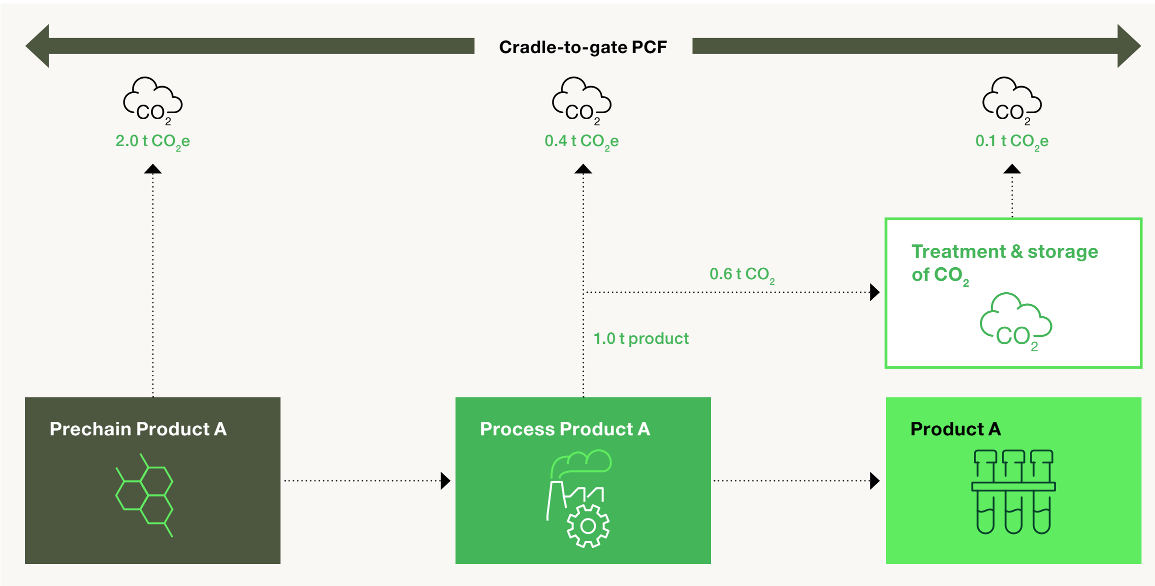
Carbon Capture and Storage

CCS may be included in the PCF calculation if a permanent and complete storage in storage facilities is guaranteed. The time frame is 100 years for permanent storage, but any leakages have to be identified, monitored, reported and considered in the PCF calculation of the product. Permanent storage technologies are characterized by a very low risk of a physical reversal of the storage process. The World Economic Forum offers a comprehensive overview of storing technologies. The net result of GHG emissions, stored GHG emissions and the deployed storage technology shall be documented. The individual amounts of emitted GHG (e.g. via capturing, transport, storage) and stored GHG could be reported separately [BASF SE (2021)]. In Table 5.12 examples are shown of CCS processes and applications, Figure 5.21 gives an overview of an example process and the PCF calculation linked to it.

Table 5.12 Examples for CCS

Example case (See figure 5.21)	Applicable PCF calculation rule	Voluntary additional information for emission offset
The company installs a facility for carbon capture and guarantees permanent and complete storage of 0.6 tons of CO_2 (CCS)	The capture of 0.6 tons of CO_2 should be considered. The net result of the PCF shall include the stored emission of 0.6 tons as well as released emissions from the capturing, any transport as well as the storage (See figure 5.21)	Absolute values of released emissions and stored emissions can be reported individually

Figure 5.21 CCS example assuming 0.6t CO_2 storage per ton product A



PCF (Product A) = 2.0 t CO_2 e/ t + 0.4 t CO_2 e/ t + 0.1 t CO_2 e/ t = 2.5 t CO_2 e/ t

CCS may only be included in the PCF if the CCS technology is active whenever the product is being produced.

Without CCS, the emission of the "Process Product A" would be 1t CO_2e, which would result in an overall emission of 3.0t CO_2e. With CCS, the emission of the "Process Product A" is lowered to 0.4t. For treatment and storage, 0.1t CO_2e are emitted; thus, the overall net CO_2e is 2.5t CO_2e (2.0t + 0.4t +0.1t)

- Net PCF including CCS (Product A) to be reported: 2.5 t CO_2e.
- Voluntary additional information on CCS: 0.6t CO_2 (captured and stored).
- Voluntary additional information on released GHG emissions: 0.4t (process) and 0.1 t (treatment).

Carbon Capture and Utilization

Captured CO_2 is a product of human transformation and can be used as a feedstock for producing chemicals (also called CCU) like waste plastic utilized in recycling. Standards for product LCAs are currently not harmonized when evaluating recycling technologies and do not fully address the steering effect of PCFs for important recycling technologies with the potential to reduce GHG emissions in the chemical industry, such as the case for CCU. Herein, a cut-off approach (also known as recycled content approach originally described in GHG protocol and discussed in this guideline chapter 5.2.8.4) commonly used for recycling is described. Thus, practitioners should use cut-off approach when calculating PCFs for CCU containing systems to harmonize the results.

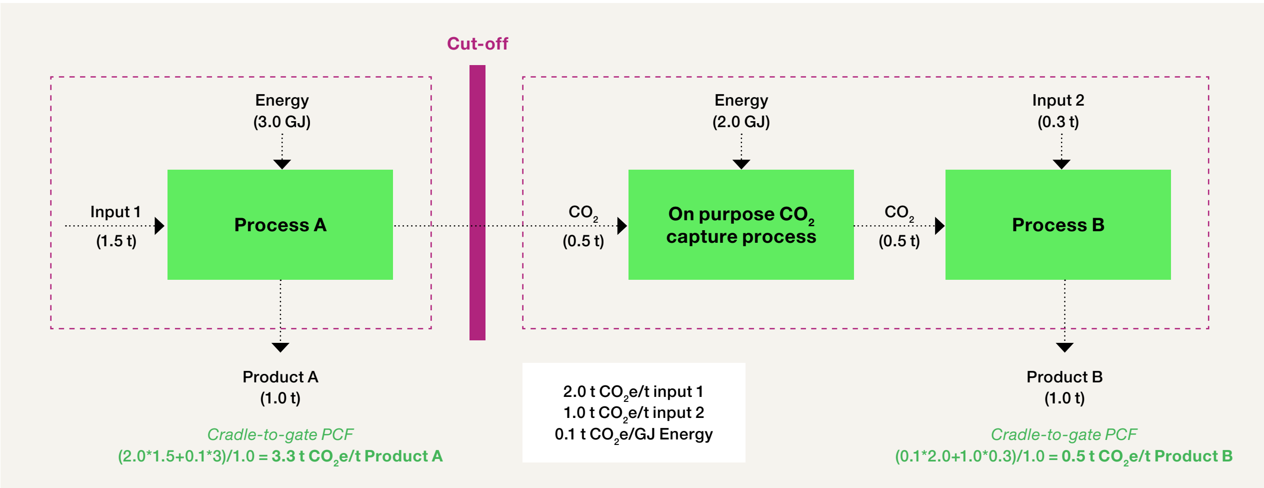
To explain the cut-off approach, an illustrative example is provided in Figure 5.22 where Process A produces CO_2 as a waste product, which is captured and used in Process B as a feedstock. The classification of CO_2 as a waste follows the decision tree in Figure 5.7. In this example, CO_2 would have been discarded if there was no CCU. Thus, a separate CO_2 capture process is needed for CCU to make product B, which require additional energy. Few examples for this type of chemical processes where CO_2 would need an additional capture unit are ethylene oxide, acrylic acid, and steam cracking process.

For the PCF calculation, the cut-off is placed before the CO_2 capture process (Figure 5.22). GHG emissions related to capture and utilization are linked to the cradle-to-gate PCF of product B (0.5 t CO_2e/t Product B), which is a sum of energy related emissions (0.1 t CO_2e/GJ * 2 GJ = 0.2 t CO_2e) and input 2 cradle-to-gate emissions (1.0 t CO_2e/t input 2 * 0.3 t input 2 = 0.3 t CO_2e). On the other hand, cradle-to-gate PCF of product A (3.3 t CO_2e/t Product A) is calculated based on input 1 emissions and energy related emissions, which is (2.0 t CO_2e/t input 1 * 1.5 t input 1 + 0.1 t CO_2e/GJ * 3 GJ = 3.3 t CO_2e). The benefits of this kind of recycling process are shared among the producing and receiving process, the 0.5 t CO_2 used in the capture process are burden-free for the user of the captured CO_2. In the case where process B and CO_2 capture are operated by separate companies, the companies shall communicate with each other regarding the partial PCF (cradle-to-gate) of the CO_2 exchanged between them.

If the CO_2 capture process is already part of Process A and is required for making proper specifications of product A (for example, water-gas-shift process in hydrogen production or acid gas removal unit in natural gas production), cut-off may be placed after CO_2 capture process. Another example of this is a power plant that is required to reduce its emissions to comply with a regulatory framework. Thus, it installs a CO_2 capture unit. If the captured CO_2 is used in Process B, then the burden of the CO_2 capture should be part of Process A.

In the CCU approach described here, only fossil and other anthropogenic captured CO_2 emissions are taken into account. If biogenic CO_2 (e.g. CCU from bioethanol fermentation) or CO_2 from direct air capture (DAC) are captured and utilized, then biogenic or atmospheric elemental carbon content stored in the product shall be

Figure 5.22 PCF calculation example for CO_2 capture and utilization where CO_2 capture requires a separate on-purpose process that is not part of Process A (e.g, ethylene oxide, acrylic acid, steam cracking process)



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reported separately as noted in chapter 5.2.10 and in the TfS Data Model. In the PCF calculation of the CCU-using product, a carbon correction shall be applied, reflecting the carbon assimilation associated with the carbon content of the product. For example, if CO_2 used in Process B is biogenic or from DAC, then CO_2 uptake shall be taken into account in the PCF calculation of Product B. Assuming Product B's CO_2 uptake is 0.5 kg CO_2e/kg product, then the final cradle-to-gate PCF for Product B with CO_2 uptake would be:

Cradle-to-gate PCF for Product B (with biogenic CO_2 uptake) = 0.5 - 0.5 = 0.0 kg CO_2e/kg product B

If biogenic CO_2 uptake is considered in Product B due to its biogenic carbon content, then this carbon cannot be counted for CO_2 uptake in Process A.

Utilization of CO_2 sources in the chemical industry is most likely based on concentrated sources of fossil CO_2, such as those from hydrogen or ethylene oxide production. PCF calculations for products based on captured CO_2 should follow the cut-off approach and CCU-based carbon content be reported separately as noted in the TfS Data Model.

In general, the CO_2 can also be derived from DAC.

If the credit approach is considered for fossil CO_2 utilization, the following model applies:

- Process A is burdened with +1 kg CO_2e for every kg of CO_2 generated
- Process B is credited with -1 kg CO_2e for every kg of CO_2 consumed from Process A.

For the credit approach, a separate external bookkeeping certification scheme shall be considered to avoid wrong interpretations and calculations along value chains. Similarly, if CCU based products are mixed with conventional versions and offered as mass-balanced products, then proper external certification schemes shall be employed as discussed in Chapter 5.2.10.5.

5.2.10.5 PCF calculation of mass-balanced products

Mass balance is a chain of custody 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 plastic 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 raw 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.

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

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 of a sustainable input[1] (feedstock, fuel, energy, etc.) to a product of interest to generate a mass-balanced PCF, 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, REDcert2, UL ECVP 2809, RSB Advanced Materials, FSC, RSPO, or equivalent). The section considers a possible chain of custody certification scheme, the mass-balancing, in detail. The chain of custody certification schemes allow a variety of system boundaries (e.g., process, plant, site, multi-site) and attribution methods.

It should be checked that the chosen sustainable input for mass balance attribution and the calculation of the required amount of the sustainable input follows the basic calculation rules as described in this guideline. Different attribution approaches can lead to differing certified sustainable shares, as this influences the qualitative MB-claim and the PCF, the attribution approach shall be transparently described in the PCF calculation. Attribution methods need to be chosen depending on the product system, made transparent, and their suitability shall be confirmed by the auditor.

(1) e.g. circular, bio or low carbon feedstocks are examples for sustainable feedstocks.

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 PCF calculation, the system boundaries for the fossil and the mass-balanced product shall follow the standards mentioned in section 5.2.4.

Biogenic carbon from the biogenic feedstock is attributed to the MB product's carbon content and its non-thermal (feedstock-related) emissions from process, waste, wastewater, and residues, leading to a PCF reduction.

For bio- or bio-circular attributed raw materials, the biogenic uptake can be considered, but double-counting shall be avoided (e.g., biogenic uptake shall be allocated in a stoichiometric way to bio-based material and potential bio-waste streams). Therefore, high attention is necessary when allocating biogenic or bio-attributed carbon. To also reflect mass-balanced products the term "biogenic carbon content" should be extended to "biogenic carbon content/attributed biogenic carbon (acc. to the mass-balance approach".

For consistency, reporting of MB product PCF should follow the requirements for reporting as defined in the TfS data model, which in turn follows ISO 14067. Specifically, the biogenic emissions and removals should be reported separately and can be integrated into the final PCF score. The biogenic carbon content and the fossil carbon content shall be reported in addition to ensure an accurate end-of-life calculation.

The mathematical approach to calculating PCF for processes in which mass balance occurs is different for different types of chemical processes.

Herein, two illustrative examples of PCF calculation methods for MB products are shown in Figure 5.23. The "inventory" calculation method is shown at the bottom of the figure, while the "conventional reference" calculation method is shown at the top-right side. Both methods describe two sets of possible balancing options. In option (1), a 50% mix of MB and conventional product is generated, and in option (2), 100% MB product is generated. Both options also generate their respective amounts of unaltered conventional products. Other mass-balancing options from 0-100% or a mix of multiple balancing options in the same system are all possible and could be calculated using either of the described methods.

In the "inventory" calculation method, conventional input A and alternative input A* are mass-allocated to a final product along with energy usage and direct process emissions based on the recipe of the process. That covers the input allocation step, labeled as Mass-allocated PCF component in Tables in Figure 5.23. Total inventory inputs, products and losses are mass-balanced. An energy content allocation could also be applied instead of a mass allocation. Then, GHG emission characteristics (labeled as "Emission factor" in Tables in Figure 5.23) of inputs are freely attributed to outputs (attribution step). In the last step, attributed emissions (calculated by multiplying the input amounts and emissions factors) are summed up and divided by the total product amount to calculate PCF of MB or conventional product. Thus, the "inventory" PCF calculation for MB product can be done using emission factor and the amount of the alternative material. This fulfills the criteria of a conventional LCA, which can be prepared as a stand-alone option without additional reference products.

Alternatively, the calculation can also be done with the information of the PCF of the fossil product. The advantage of this approach is that all the process utilities usage, thermal emissions, etc,. are already included in the PCF of the fossil product and do not have to be assessed separately.

In the "conventional reference" PCF calculation method, the PCF for MB product can also be calculated with the information from the PCF of the conventional product using the following formula (also noted in the Figure 5.23):

Formula 5.3

$$\text{PCF (Product x\% MB)} = (\text{PCF}_{conventional} * \text{Mass}_{output} + \text{effect from feedstock replacement}) / \text{Mass}_{output}$$

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Figure 5.23 Mass Balance – Illustrative examples of PCF calculation methods

100 t of Conventional inputs(1)
3.0 t CO_2e/t

+25 t Input A*
1,0 t CO_2e/t

-25 t fossil Input A
3.0 kg CO_2e/t
(=> 75 t conventional + 25 t sustainable feedstock)

Partial substitution of conventional inputs

25 t input A replaced by 25 t sustainable feedstock A*:

Certified that 25 t A replace 25 t A and attribution of input A* to Product is allowed*

(1) Single or multiple inputs

Mass balance Attribution

25 t Sustainable Characteristics

(PCFA* - PCFA)* 25t
= -50 t CO_2e

Production: 45 t CO_2e emissions, 180 GJ heat (0.1 t CO_2e/GJ), 10 t production losses
(2) Mass Balance Inputs

100 t Inputs
313 t CO_2e(2)

Exemplary options for Outputs following Mass Balance system

Calculation Method "Conventional reference"

PCF (Product$_{x\%\ MB}$) = (PCF$_{conventional}$ * Mass$_{output}$ + effect from feedstock replacement) / Mass$_{output}$

1

-50 t CO_2e

MB 50%
45.0 t
2.9 t CO_2e/t

PCF (Product$_{50\%\ MB}$)
= (4.0 t CO_2e/t * 45 t
+ 25 t * (- 2 t CO_2e/t) / 45 t
= 2.9 t CO_2e/t Product

Conventional product
45.0 t
4.0 t CO_2e/t

90 t Products | 10 t Losses | 313 t CO_2e

2

-50 t CO_2e

MB 100%
22.5 t
1.81 t CO_2e/t

PCF (Product$_{100\%\ MB}$)
= (4.0 t CO_2e/t * 22.5 t
+ 25 t * (- 2 t CO_2e/t) / 22.5 t
= 1.8 t CO_2e/t Product

Conventional product
67.5 t
4.0 t CO_2e/t

90 t Products | 10 t Losses | 313 t CO_2e

Calculation Method "Inventory"

1

MB 50%
45 t
2.9 t CO_2e/t

Mass-allocated PCF component	Emission factor	Emissions
Input A*, 25 t	1.0 t CO_2e/t input A*	25 t CO_2e
Input A, 25 t	3.0 t CO_2e/t input A	75 t CO_2e
Heat, 90 GJ	0.1 t CO_2e/GJ heat	9.0 t CO_2e
Emission, 22.5 t CO_2	1.0 t CO_2e/t CO_2	22.5 t CO_2e
MB 50% Product, 45 t	**131.5/45 = 2.9 t CO_2e/t product**	**131.5 t CO_2e**

Conventional product
45 t
4.0 t CO_2e/t

Mass-allocated PCF component	Emission factor	Emissions
Input A, 50 t	3.0 t CO_2e/t input A	150 t CO_2e
Heat, 90 GJ	0.1 t CO_2e/t GJ heat	9.0 t CO_2e
Emission, 22.5 t CO_2	1.0 t CO_2e/t CO_2	22.5 t CO_2e
Fossil product, 45 t	**181.5/45 = 4.0 t CO_2e/t product**	**181.5 t CO_2e**

90 t Products | 10 t Losses | 313 t CO_2e

2

MB 100%
22.5 t
1.8 t CO_2e/t

Mass-allocated PCF component	Emission factor	Emissions
Input A*, 25 t	1.0 t CO_2e/t input A*	25 t CO_2e
Heat, 45 GJ	0.1 t CO_2e/GJ heat	4.5 t CO_2e
Emission, 11.3 t CO_2	1.0 t CO_2e/t CO_2	11.3 t CO_2e
MB 100% Product, 22.5 t	**40.8/22.5 = 1.81 t CO_2e/t product**	**40.8 t CO_2e**

Conventional product
67.5 t
4.0 t CO_2e/t

Mass-allocated PCF component	Emission factor	Emissions
Input A, 75 t	3.0 t CO_2e/t input A	225 t CO_2e
Heat, 135 GJ	0.1 t CO_2e/GJ heat	13.5 t CO_2e
Emission, 33.8 CO_2	1.0 t CO_2e/t CO_2	33.8 t CO_2e
Fossil product, 67.5 t	**272.3/67.5 = 4.0 t CO_2e/t product**	**272.3 t CO_2e**

90 t Products | 10 t Losses | 313 t CO_2e

The PCF of the MB product is calculated by adding the effect of the feedstock substitution (delta PCF between alternative and conventional feedstock multiplied by the certified amount of replaced feedstock) to the conventional product's total emission. The resulting emission is then divided by the volume of the MB product. The volume threshold is set by the certified amount of conventional feedstock replaced by sustainable input, including losses.

The method ensures that the PCF is calculated by replacing the impact of the conventional raw material with the sustainable input, in the amount that is exchanged. This results in a linear relationship between degree of feedstock substitution and PCF reduction, while the emissions of the conventional systems remain considered. The feed-in point of the sustainable input determines the substituted comparable conventional feedstock. In any case, for the PCF calculation, a check is carried out to ensure that the amount of renewable and recycled carbon does not exceed the sum of the amount of carbon in the product plus the amount of carbon in the feedstock-associated emissions.

Additionally, this approach ensures the comparability of the fossil and MB PCFs. Following the certification schemes a specific amount of sustainable input is procured and used in the production. The PCF for mass-balanced products is calculated by replacing the impact of the conventional raw material in the amount that is exchanged by the sustainable input (see 4.6.7.1.1).

As one published example, Jeswani [Jeswani et al [2019]] described a methodology for integrating the mass balance approach into LCA for biomass applications in the chemical sector. The concept conforms to the requirements of ISO 14044 [ISO 14044: 2006] and may be applied to mass balance applications using bio-based feedstocks (biomass balance). The number of sustainable feedstocks required to replace the fossil inputs are calculated through material flow analysis. The life cycle inventory of outputs with attributed sustainable content (using mass balance) is determined based on relative conversion rates of the different feedstocks and chemical values of the resulting outputs.

For both calculation methods, if the circular feedstock is known to change the energy use and direct emission outputs or the efficiency of the system, this shall be considered.

Multi-input single-output systems necessarily need different raw materials with different footprints to produce the desired output. Via the free attribution approach, MB accounting allows attribution of the bio-based or recycled characteristics from one input to the whole molecule of the single output (mass of input equals mass of output multiplied by a conversion factor). There is a certain risk that a raw material with a low footprint is used to be attributed to the output share, while the higher footprints of the other raw materials are neglected. Therefore, it shall be transparently documented which approach was used.

5.2.11 Data quality and share of primary data

5.2.11.1 Share of primary data

To create visibility on the share of primary data in PCF calculations, the primary data share (PDS) in each dataset shall be determined (and shared) [PACT Methodology]. 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 GHG impact (CO_2e) that is derived by using primary data in the cradle-to-gate system boundary (see Formula 5.4). In the exceptional case where a PCF contribution is zero, this formula cannot be applied.

See glossary for definitions of primary and secondary data.

Formula 5.4: Calculation approach of the PDS

$$PDS_{DU} = \frac{\sum(|IC_i| * PDS_i) + (BCC * 44/12 * PDS_{BCC})}{\sum|IC_i| + BCC * 44/12}$$

Where:

- DU is the declared unit
- PCF_{DU} is the product carbon footprint of the DU excluding biogenic CO_2, in kg CO_2e/DU
- PDS_{DU} is the primary data share of PCF_{DU}, in % (0-100%)
- i is any input or output of a process, except the DU
- $|IC_i|$ is the absolute value of the impact contribution of i to PCF_{DU}, in kg CO_2e/DU
- PDS_i is the primary data share of contributor i, in % (0-100%)
- BCC is the biogenic carbon content of the DU, as fraction of DU
- PDS_{BCC} is the primary data share related to the BCC (typically 100%)

Note 1: The factor 44/12 converts carbon content of CO_2 based on molecular masses of CO_2 (44) and C (12).

Note 2: If every IC_i is greater than zero, $\sum|IC_i|$ will be equal to PCF_{DU}.

The contribution of biogenic carbon is included in this formula to address the contribution of bio-based materials to the PDS, even if the PDS is often 100% when the BCC is known.

Ideally, the share of primary data for relevant input flows obtained from upstream suppliers (tier n-1) should be available. If so, the PDS of the PCF is calculated using a PCF-attributed average approach of the material and energy inputs. All members of the supply chain are encouraged to participate in this effort. However, the share of primary data can only be accurately determined if the information for most inputs is provided by the respective suppliers.

Figure 5.24 Calculation of Primary data shares of two fossil components

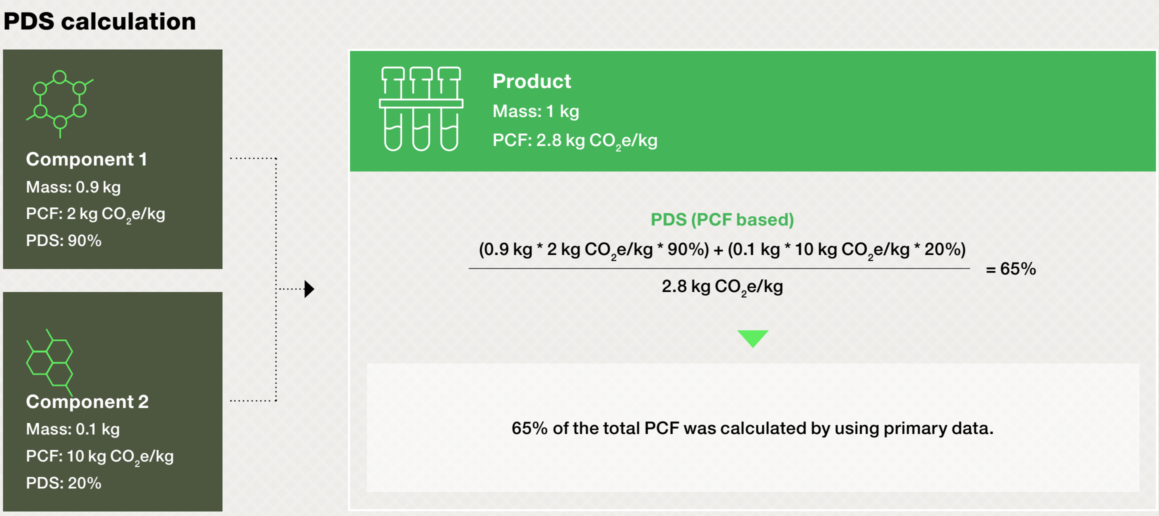
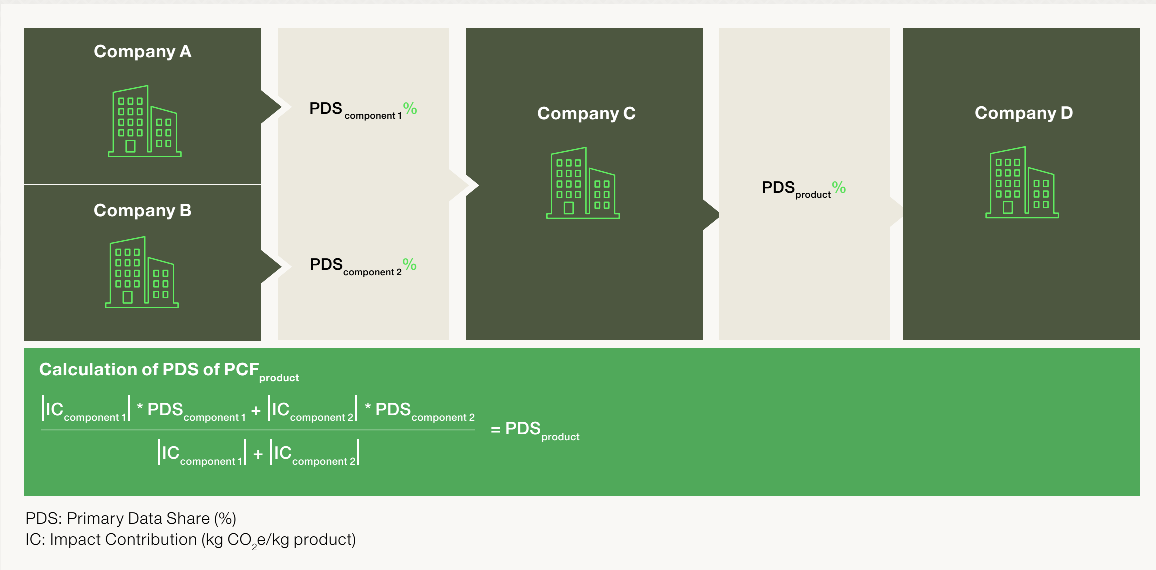


Figure 5.25 Calculation of Primary data share for a PCF [PACT Methodology]



To calculate the total PDS, the individual PDS received from suppliers as well as from other components, e.g., energy inputs or direct emissions from production, are multiplied against the ratio of their respective relative impact contributions (in absolute value) to the sum of absolute values of each impact contribution. All these weighted PDS components are then added up to obtain a total PDS of the declared unit.

To increase the transparency on primary data use, information on PDS shall be shared downstream (tier n+1) together with the PCF, as described in the data exchange format. The inclusion of an explanation for the share of primary data is thus encouraged, with the objective of helping businesses support each other in increasing the amount of primary data flowing through the system. This ensures more accurate PCFs, particularly when the quality of the data is very good (Figure 5.24). The approach of PACT in the published version is shown in Figure 5.25.

Figure 5.26 Example of calculation of the Primary data share for a fossil PCF (left column) and for a PCF including biogenic carbon (right column)

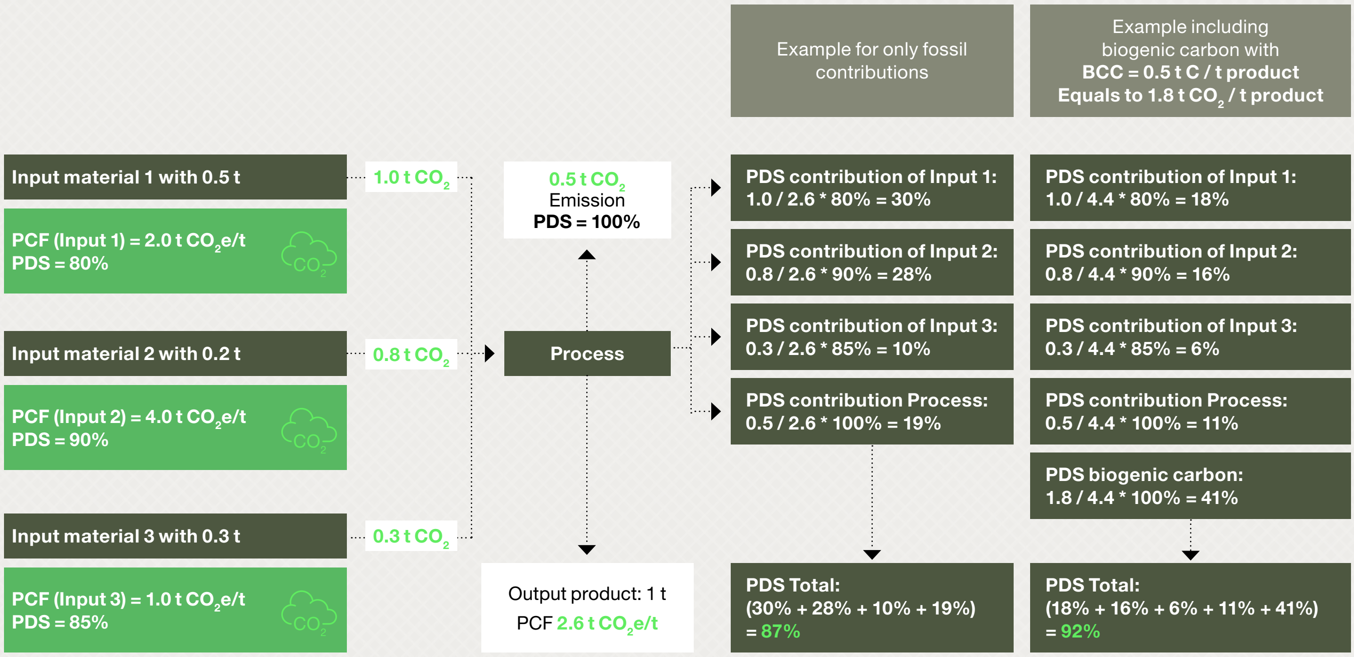


Table 5.13 PDS calculation example for primary and secondary data sources

Material	Data input (respective units)	Data source	EF (kg CO_2e/ unit)	EF source	Impact contribution (kg CO_2e)	PDS
A	10,435	Primary	0.19	Primary	1,983	100%
B	10,000	Secondary	0.18	Secondary	1,800	0%
C	5,000	Primary	0.18	Secondary	900	0%
Product	**1**				**4,683**	**42%**

A detailed example is shown in Figure 5.26, demonstrating the application of detailed steps in generating a PDS for a PCF of a product. A primary data share shall only be attributed if both the activity data (e.g., amount in kWh) and the emission factor information are derived from primary sources. If either of these is derived from secondary data, the PDS for this unit process is rated as secondary data, i.e., PDS = 0%, see a related example in Table 5.13.

The PDS shall be calculated for PCF including all biogenic emissions and removals. The biogenic CO_2 emissions can be omitted as they are balanced with the assimilation. For biogenic materials, their contribution is calculated using their biogenic carbon content (BCC), which can be transferred to CO_2 using the ratio of molecular masses of CO_2 (44) and C (12). The PDS of this element is often 100% because the BCC is a known figure and shall be reported in the TfS data format. In the example on Figure 5.26, if the produced product is bio-based with e.g., 50% BCC, it results in a CO_2 figure of 0.5 * 44/12 = 1.83 kg CO_2. This leads to new PDS figures shown in the rightmost column of Figure 5.26.

5.2.11.2 Data quality rating

During the data collection process, companies shall assess the data quality of PCF impact contributors (emission factors and/or direct emissions data) by using the data quality indicators (DQIs). The data quality of each PCF 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 data quality rating (DQR) following the criteria outlined in this chapter. Data sourced from verified emission factor databases (see chapter 5.2.6) 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 PCFs issued from 2027 onwards, giving companies sufficient time to prepare. Until then 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 standard were harmonized with PACT Methodology, Catena-X and GBA. Three DQIs are required for the assessment of data quality; this change with respect to the previously issued guideline will also be reflected in version 3 of the PACT Methodology.

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 and should also use the same matrix proposed for emission factors. The rationale behind this approach is as below:

- **Overlap with existing approaches:** Focusing on the assessment of emission factors and direct emissions only is consistent with all approaches that are currently available.
- **Mitigation of complexity:** Assessing emission factors quality and direct emissions only limits potential complexities introduced in a new approach (for activity data quality) as, in practice, assessing activity data quality and emission factors quality is quite different (e.g., single matrix descriptions are not fully applicable for both data types).
- **No additional assessment of activity data:** All guidance request to have primary activity data and therefore, technology, geography and temporal DQRs will result in '1 - Excellent' most of the time. Similarly, whenever direct emissions are not estimated through proxies but directly measured, their associated DQR will also result in '1 – Excellent' in most cases.
- **Practicality and scalability:** Having a simple solution, that is used across industries, is essential to enable companies to adopt this metric for all their products.

The quality indicators are summarized in Tables 5.14-5.16.

- **Technological Representativeness (TeR):** the degree to which the data reflect the actual technology(ies) used in the process.
- **Geographical Representativeness (GeR):** the degree to which the data reflect 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 reflect the actual time (e.g., year) when the process was assessed.

The quality assessment of data based on the Tables 5.14 to 5.16 can be used to derive more quantitative information in form of a DQR to give users of the data a better impression of the overall quality of data and the resulting PCF. The quality levels 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.

Regarding the assessment of the single indicators, and especially regarding technology representativeness, note that any data from a supplier that is not taken "as is" and used for its original purpose should be reassessed according to the Tables 5.14 to 5.16. Notably, if a supplier's PCF for a product A is not used to represent the exact product A supplied to our process but it is used instead to approximate a product B from a different supplier, this counts as a proxy and should automatically imply a reassessment of the DQR with a rating for technological representativeness between 3 and 5. The same reasoning can hold for geographical representativeness.

The aggregation of the three indicators into a single DQR happens at the level of each input/output material, i.e., emission factor or direct emission. The DQR of each input/output material corresponds to the average of the three data quality indicators, assuming equal weights for each criterion (see also equation marked as first line in Formula 5.5). An example of this process is described below for two generic products A and B.

For example:	**Product A**	**Product B**
Technology Representativeness (TeR)	2	3
Temporal/Time Representativeness (TiR)	1	3
Geography Representativeness (GeR)	2	2
Total	**5**	**8**
DQR Process (Total / 3)	**1.7**	**2.7**

The PACT Methodology requires only those inputs representing more than 5% of the sum of absolute values of each impact contribution to undergo the DQR assessment which reduces the workload for the generation of DQR factors. TfS recommends this approach as well.

Table 5.14: Overview of criteria of the assessment of the technology representativeness

1	2	3	4	5
The dataset has been created based on data reflecting the exact technology employed (i.e. plant specific process/equipment data for the plant/equipment where the product has been manufactured)	The dataset has been created based on data reflecting the company-specific and same technology to the one employed for the actual manufacturing (i.e. same technology, the company/site specific but not necessarily plant specific – it could be an average if several company/site specific data are available)	The dataset has been created based on data reflecting an average for an equivalent technology to the one employed for the actual manufacturing (i.e. same technology, but not company specific)	The dataset has been created based on data reflecting a technological proxy (i.e. similar but not same technology, irrespectively if based on averages or supplier-specific data)	The dataset has been created based on different or unknown technology vs technology actually employed
Explanation: *This quality score can be achieved only in case of use of primary data*	*Explanation:* *This quality score can be achieved only in case of use of primary data*	*Explanation:* *This is the maximum score achievable with secondary data*		

Table 5.15: Overview of criteria of the assessment of the geography representativeness

1	2	3	4	5
The dataset has been created based on data reflecting the country subdivision (if applicable) or country in which the product has been manufactured	The dataset has been created based on data pertaining the country, (when country subdivision is applicable), in which the product has been manufactured. The area where the dataset is generated is valid for the geographical area where the site is located	The dataset has been created based on data pertaining the geographical region (e.g. Europe, Asia, N. America), in which the product has been manufactured. The area where the dataset is generated is valid for the geographical area where the site is located	The dataset has been created based on global averages	The dataset has been created based on data with a geographical scope which is either unknown or pertaining a country, or region not including the site in which the product has been manufactured
Example for country subdivision: *Provinces in China, States in the US,* ***federative units in Brazil,*** *etc. applicable for bigger countries*	*Example:* *The site is in California and the dataset is a US average*	*Example:* *The site is in Spain and the dataset is a European average*	*Example:* *The site is in Japan and the dataset is a global average*	*Example 1:* *In absence of a global average, the dataset geographical applicability is unknown.* *Example 2:* *The site is in Mexico, but the dataset is a US average, or a Finnish average or an Asian average or a European average*

Table 5.16 Overview of criteria of the assessment of the temporal/Time representativeness

1	2	3	4	5
The difference between “Reference Period End” of the dataset and “Date of Issue” of the PCF is ≤1 year (i.e. 366d (to count for leap year))	The difference between “Reference Period End” of the dataset and “Date of Issue” of the PCF is >1 year and ≤2 years (i.e. 731d)	The difference between “Reference Period End” of the dataset and “Date of Issue” of the PCF >2 years and ≤3 years (i.e. 1096d)	The difference between “Reference Period End” of the dataset and “Date of Issue” of the PCF is >3 years and ≤4 years (i.e. 1461d)	The difference between “Reference Period End” of the dataset and “Date of Issue” of the PCF is >4 years

“Reference Period End”* (e.g., data collected between 01.01.2023-31.12.2023)
“Date of Issue”** (e.g. 01.06.2024)
Calculate Time Difference: “Reference Period End” – “Date of Issue” (e.g. 31.12.2023 - 01.06.2024) = 6 months, i.e. rating 1

* Data collection end period

** The time stamp at which the PCF has been released for communication, independently of when or if it has been shared.

In Formula 5.5, the first equation shows the general calculation of a single DQR of an input or output material, based on the three DQIs described above. In the second equation is shown the aggregation of DQRs of each impact contributor into a total DQR score of the PCF of a declared unit.

DQR shall be calculated for PCF including all biogenic emissions and removals. The PCF is calculated with the absolute value of PCF contributions |IC| to accurately include negative impact contributors.

The contributions of the input materials to the PCF of the process are linked with the DQR of the input material. The closer to 1 the DQR score (higher quality) and higher the share of the impact contribution, the more positive is the effect of an input material to the overall DQR score.

Formula 5.5: General calculation of data quality ratings

$$DQR_i = \frac{TeR_i + GeR_i + TiR_i}{3}$$

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

$$DQR_{DU} = \frac{\sum (|IC_i| * DQR_i) + BCC * 44/12 * DQR_{BCC}}{\sum |IC_i| + BCC * 44/12}, \text{ for } |IC_i| \geq 0.05 \sum |IC_i|$$

Where:

- DU is the declared unit
- PCF_{DU} is the product carbon footprint of the DU excluding biogenic CO_2, in kg CO_2e/DU
- DQR_{DU} is the data quality of PCF_{DU}, in range 1-5
- i is any input or output of a process, except the DU
- $|IC_i|$ is the absolute value of the impact contribution of i to PCF_{DU}, in kg CO_2e/DU
- DQR_i is the data quality of contributor i, in range 1-5
- BCC is the biogenic carbon content of the DU, as fraction of DU
- DQR_{BCC} is the data quality related to the BCC

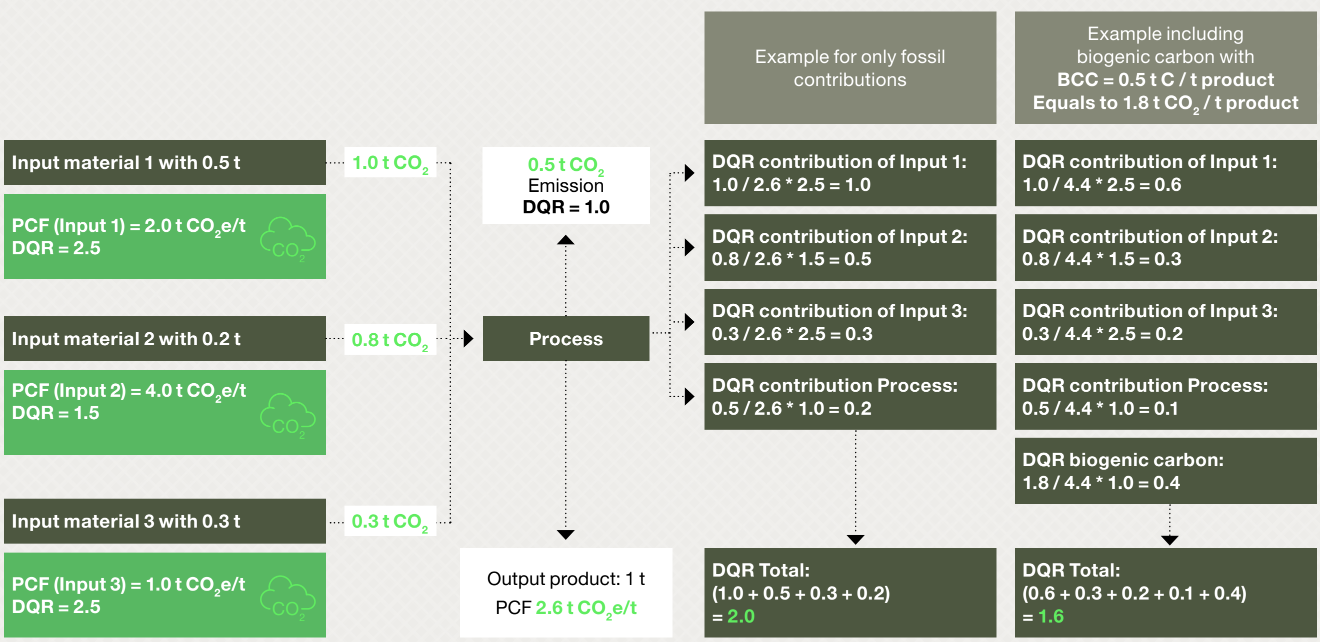
Note 1: The factor 44/12 converts carbon content of CO_2 based on molecular masses of CO_2 (44) and C (12).

Note 2: If every $|IC_i|$ is greater than zero, $\sum |IC_i|$ will be equal to PCF_{DU}.

Note 3: Since DQR_i is a linear combination of DQIs, replacing DQR_i in the main equation with either TeR_i, GeR_i or TiR_i will yield the respective value of a DQI for DU.

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

Figure 5.27 DQR example for a process including upstream DQR



For an example, see Figure 5.27, the total DQR for this process is 2.0 and shall be reported to the recipient of the PCF data as well after end of 2027. Similarly, the same total DQR for a process with bio-based product (assuming a BCC of 50%) is 1.6. In the example shown, the DQR of the biogenic contribution was assumed equal to 1, since entirely calculated from primary data.

The DQR can be used as an input for complete LCA, which enables the final calculation of a complete DQR. The DQR supports the interpretation of PCF data and supports the identification of improvement potentials of the quality of the PCF data.

Improving data quality

Collecting data and assessing its quality is an iterative process for improving the overall data quality of the product inventory. If data sources are identified as low quality using the data quality indicators, companies should recollect data [GHG Protocol Product Standard].

The following steps are useful when improving data quality:

1. Identify sources of low-quality data in the product inventory using the data quality assessment results. Sources with low quality data that have been identified as significant to the PCF results should be given priority.

2. Collect new data for the low-quality data sources as resources allow.

3. Evaluate the new data. If it is of higher quality than the original data, use in its place. If the data are not of higher quality, either use the existing data or collect new data.

4. Repeat as necessary and as resources allow. If companies change data sources in subsequent inventories, they should evaluate whether this change creates the need to update the base inventory.

5.3 Verification and reporting

5.3.1 Verification of PCF calculations and certification of PCF programs or companies

Various Stakeholders, including customers, investors, and regulators, rely on Product Carbon Footprint (PCF) data to make informed decisions about sustainability and climate action. Without trust in the reported PCF results, stakeholders may be skeptical of the claims made by companies and may question the effectiveness of sustainability efforts. Thus, building trust in PCF results is essential for ensuring that sustainability efforts are credible and effective.

A new document of TfS and Catena X was prepared to give guidance on verification and certification processes and requirements. The "Catena-X and TFS PCF Verification Framework" document is accessible at the following link for further reference on this topic: **https://www.tfs-initiative.com/how-we-do-it/scope-3-ghg-emissions/pcf-guideline#verification-framework.**

As a short summary of the framework, three levels of trust are defined:

Level 1: PCF Dataset Check
Level 2: PCF Program Certification
Level 3: PCF Verification

Trust Level 1 is a completeness check, including conformity with the PCF data model, and is often performed in automated fashion through data exchange platforms and connected solutions. It does not constitute a certification or verification.

Trust Level 2 is a 3rd party attestation related to a conformity assessment of a company's PCF program. It entails a certification of the company's application of PCF calculation tools.

Trust Level 3 refers to the verification of the specific PCF dataset, defined as process for evaluating the PCF information statement based on historical data and information to determine whether the statement conforms with the TfS PCF Guideline.

Verification should be the standard approach for TfS-compliant PCFs. The verification shall be performed by an independent party, which can be a 3rd party, or alternatively, a 1st or 2nd party acting as a verifier. The trust level associated with 1st or 2nd party verification is lower than that of 3rd party verification. A verification conducted by a 1st or 2nd party comes with the precondition of an existing PCF program certification.

In the case of a 2nd party verification, the 2nd party (i.e., the customer) would request and be granted access to additional data on top of the regular PCF data model from the supplier to enable an expert judgement on the plausibility of the exchanged PCF. A pre-condition of a 2nd party verification is a valid PCF program certification of the supplier (i.e. trust level 2). Moreover, the parties may sign a non-disclosure agreement about the additional data exchange. With such condition fulfilled, the 2nd party shall request confidential access to the following additional data (as a minimum requirement):

- Location of production,
- declaration of supplier type (e.g. manufacturer or distributor),
- adoption of specific PCRs in the PCF calculation,
- other data which are included in the PCF data model, but have not yet been provided, because declared as "optional" or not yet "mandatory" at the time of the PCF exchange,
- manufacturing technology employed.

The type of verification shall be reported together with the PCF; more details are provided in the mentioned framework. The competence requirements which shall be fulfilled by a verifier/certifier or by a verifier/certifier team are published in ISO 14066:2023 chapter 4.

Additionally, the verifier shall have knowledge about and experience with:

- PCF calculation processes according to the rulebooks and underlying standards,
- The assurance levels (regular & in-depth) as defined in this framework,
- GHG emission factor sources,
- Life Cycle Assessment (LCA) and/or Product Carbon Footprinting (PCF),
- PCF verification processes according to this rulebook containing but not limited to: Strategy analysis, Risk assessment, verification planning and documentation, review procedures to ensure quality,
- Concept of materiality,
- Sector/industry/product specifics like typical production processes, monitoring techniques, typical internal control systems, applicable assumptions, best practice, GHG emissions,
- Modelling software or automated calculation solutions.

Verification of carbon offsets are out of scope of this document and the verification guideline as well. As the PCF's reporting scope is always cradle-to-gate, it is the client's responsibility to report cradle-to-gate PCF values to the customer. In case the client organization is in charge of its own outbound logistic, it shall also take care of the calculation and verification of the emissions for this relation.

The verification statement constitutes the link between the PCF dataset and the completed verification process. It indicates that the PCF dataset attributes have been verified according to a specific verification type. The verifier issues the verification statement to the client. The client can present the verification statement to the receiver of the PCF dataset (customer) with the intention to create trust in the PCF dataset. Hence, the verification statement can complement the exchange of PCF datasets.

The process of PCF program certification aims at certifying that the company calculating PCFs has established a PCF program in line with the TfS PCF Guideline. The PCF program shall include a description of the methodology used by the company to calculate PCFs. If applicable, the deployment of any automated

PCF calculation solution (tool and integrated data sources and IT management) is also subject to certification. An automated PCF calculation solution is defined as a digital tool enabling mass calculations of PCFs in an automated manner.

The guidelines do not mandate any PCF program or an automated PCF calculation solution. It is in the interest of the individual companies to adopt a company-specific approach, which is in line with the calculation rules in the respective rulebook.

The scope of the certification shall be clearly defined (e.g., organizational units, products, product groups, sites). The PCF program certification shall ensure that the methodological requirements set out in the respective rulebook are followed, including the respective mandatory attributes in the respective PCF data model.

Certified PCF programs and automated PCF calculation systems shall include a process for the PCF dataset check. In addition, the elements of the PCF program described shall be ensured. The PCF program certification shall only be used for systems, processes and calculation solutions deployed within a given company and reflecting this company's unique situation.

The certification does not certify any specific PCF dataset for a product, nor does it claim any output (e.g., a specific PCF result or dataset) of a tool or program as certified, verified or in any other way assessed. Calculations and data issued from certified PCF programs may be used as inputs to PCF verification activities. If the PCF program or automated calculation solutions are already certified and therefore known and trusted, individual PCF verification activities may build on this and therefore be simplified. A PCF program certification is mandatory to obtain a 1st or 2nd party verification. However, a PCF program certification is not mandatory to obtain a 3rd party verification of a specific PCF dataset. PCF program certifications cannot be substituted by existing certification schemes like ISO 9001 or ISO 14001.

5.3.2 Quality assurance

Quality assurance is defined as part of quality management focused on providing confidence that quality requirements will be fulfilled. In this sense, a quality assurance shall address whether the PCF results and the approach to achieve them fulfill requirements of high quality beyond data quality (adapted from [ISO 9000: 2005]).

The following short checklist can help the LCA practitioner to validate the PCF. In addition to the LCA expert, individuals who can support the validation include technology experts, controllers, plant managers, and site managers:

- Check the overall mass balance (includes raw material inputs, product outputs, wastes, and emissions into air and water).
- Check completeness of life cycle stages.
- Check the elementary balance by doing a stochiometric calculation.
- Check if direct emissions are realistic (e.g., by carbon balance).
- Check whether the carbon balance is closed: all inputs are considered and balanced with outputs to products, emissions (air, water, soil), and wastes. Check plausibility of process related direct emissions: carbon, nitrogen input-output flows are balanced out.
- Check data aggregation, data enhancement and underlying modeling to calculate product inventory of your own data sets.
- Check if correct calculation formulas were applied.
- Check if utility consumption is plausible.
- Check allocation factors (in line with chapter 5.2.9): the sum of the allocated inputs and outputs of a unit process equals the inputs and outputs of the unit process before allocation, and allocation factors over all co-products of one multi-output process sum up to 1.
- Benchmark CO_2e against own calculations, same product from other sites/plants/companies, existing LCA data, and other third-party databases.
- Check if biogenic emissions and uptakes are correctly considered and reported (5.2.10.1).
- Check the appropriateness of the secondary datasets selected for Scope 3 upstream data:
  - Check if technology and geography represented in the LCI are appropriate.
  - Check if the application of proxies is appropriate.
  - Check if dataset is replaced when supplier data becomes available.
- Check if a data quality score was generated and if it is meaningful.
- Check significant deviations from benchmarked LCA data:
  - Perform sensitivity analysis and quality checks of results: Apply different modeling choices (e.g., another dataset for a raw material, another allocation method for the foreground product system) to test the robustness of the result.
  - A variation of 10% in the PCF result (including or excluding life cycle stages) is generally accepted by practitioners due to inherent uncertainties, variabilities of factors, or data sets used in a PCF calculation. Any decisions shall be clearly stated in the internal PCF calculation report, and the reasons and implications of inclusion/exclusion shall be explained. The threshold for significance shall be stated and justified.

Any additional information available, such as a PCF report or a critical review statement, can be added to complement with more details the provided information [BASF SE (2021)].

Results reported in the PCF study report may be used in footprint communications [ISO 14026: 2017].

5.3.3 Information for reporting PCF data and additional context

Information beyond the PCF value is needed to support the interpretation and validation of PCF data, as well as to provide necessary information for quantification of customer PCFs further down the value chain. Some examples of different approaches for reporting are provided in Table 5.17.

The PCF covers one environmental impact. In this context, it should be mentioned that no overall statements on the environmental performance of the product can be made, nor are possible comparative assertions claiming the environmental superiority of one product over another. Comparisons of PCF are only possible under certain criteria if all relevant information is reported.

The "TfS PCF Data Model: How to report PCF data" document describes the data model aspect according to which PCF data shall be exchanged in compliance with the Product Carbon Footprint Guideline for the Chemical Industry of Together for Sustainability. It supersedes Table 5.20, section 5.3.2 in version 2.0 of the same guideline, and in all following versions it will be managed as a separate cross-referenced document.

The fields marked as “mandatory” in the table shall be provided by suppliers when disclosing PCF values. Some fields will become mandatory for PCFs issued from 2027 onwards to provide a transition period for adaptation. TfS still highly recommends reporting as much data as possible. Additional details, currently not mandatory, may also be provided if available, to offer further support.

ISO 14067 [ISO 14067: 2018] describes requirements for reporting, which are reflected in the attributes list. For a PCF study to be fully compliant, all reporting requirements shall be addressed.

TfS uses the data exchange platform SiGreen. The list of data attributes is published separately and will be updated independently of the update cycles of this guideline. The data exchange format can be found at: **https://www.tfs-initiative.com/pcf-guideline #tfspcfdatamodel**

Table 5.17 Reporting examples in different approaches of companies

Example case	Applicable PCF calculation rule	Voluntary additional information for emission offset
The company purchases emission credits from a project investing in reforestation to offset 50% of the calculated PCF	The PCF remains the same as calculated	The emissions offset of 50% may be provided separately from inventory results
The company purchases emission credits from a carbon capture and storage facility to offset 30% of the calculated PCF	The PCF remains the same as calculated	The emissions offset of 30% may be provided separately from the inventory results
The company purchases renewable electricity certificates to offset 100% of the electricity consumption of a particular site, and as a consequence, reduces to zero the electricity-related emissions of the PCF	The PCF is reduced according to the reduction potential of electricity use; offsets are not taken into account as credits	The emission offset may be provided separately from inventory results
The company generates direct CO_2 within a reaction, which is captured and sold as a by-product (see Chapter 5.2.10.4)	The impact of the process capturing atmospheric CO_2 and selling it as a by-product shall be added to the inventory results of the PCF according to the amount of CO_2 captured, and may be subtracted from the inventory results of the process	As an alternative to subtracting the CO_2 emissions captured and sold from the inventory results, the emissions captured may also be provided separately

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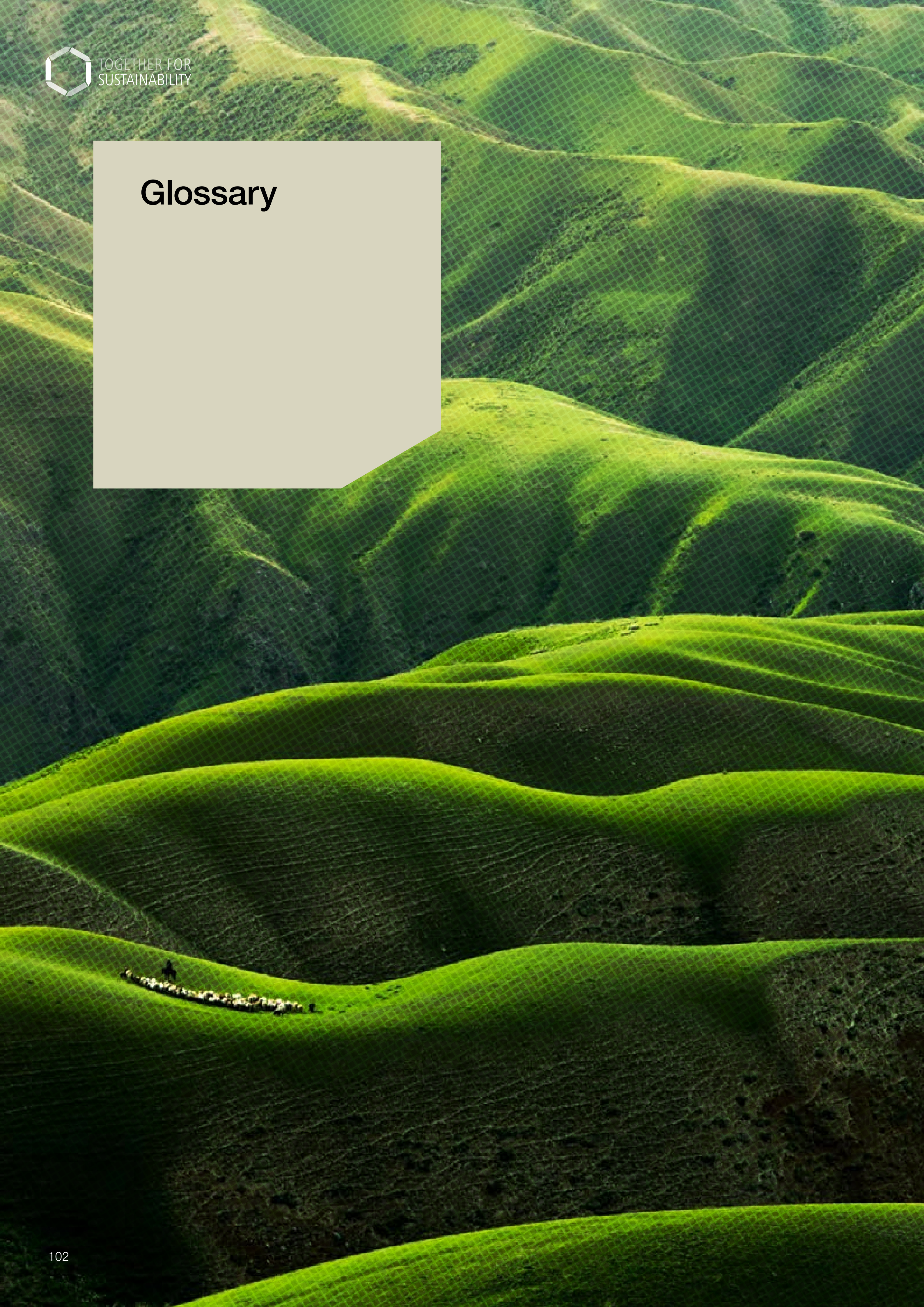

Abbreviation	Term	Definition
	Activity data	"Activity data are quantified measures of a level of activity that results in GHG emissions or removals"[1]. Activity data can be measured, modeled, or calculated. There are two categories of activity data: process activity data and financial activity data. 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.
	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.
	Background data	See also secondary data. Data that concern processes outside the operational control of the company.
	Bill of materials (BOM)	A structured list of all the components, and their quantities that make up an assembly or product.
	Biogenic carbon content	Fraction of carbon derived from biomass in a product.
	Biogenic emissions	CO_2 emissions from the combustion or biodegradation of biomass.
	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.
	Biomass	Material of biological origin excluding material embedded in geological formations and/or fossilized.
CAS number	Chemical Abstracts Service Registry Number	See table 4.2
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.
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.
CFP	Carbon footprint of a product	See Product Carbon Footprint (PCF).
CFCs	Chlorofluorocarbon	See Greenhouse Gas definition.
CH_4	Methane	See Greenhouse Gas definition.
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.
	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.
	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 from the ground and processed through each subsequent stage of manufacturing, transportation, product use, recycling, and ultimately, disposal.

Glossary

(1) https://ghgprotocol.org/sites/default/files/standards/Product-Life-Cycle-Accounting-Reporting-Standard_041613.pdf

Abbreviation	Term	Definition
	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
	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.
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.
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.
	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.
DUNS	Duns and Bradstreet Number	The Dun & Bradstreet D-U-N-S Number is a unique nine-digit identifier for businesses.
ECICS	European Customs Inventory of Chemical Substances	See table 4.2
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.
EF	Environmental Footprint	It is a multi-criteria measure to calculate the environmental performance of a product, service or 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.
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.
EU	European Union	The European Union is a supranational political and economic union of 27 member states that are located primarily in Europe.
	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.

Abbreviation	Term	Definition
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 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 (SF_6) • Nitrogen trifluoride (NF_3) 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.
GLO	Global	
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.
HCFCs	Hydrochlorofluorocarbon	See Greenhouse Gas definition.
HEFs	Fluorinated ethers	Liquid Chemical.
HFCs	Hydrofluorocarbons	See Greenhouse Gas definition.
HS	Harmonized Commodity Description and Coding Systems	See table 4.2
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.
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.
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.
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.
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 consistent with International Standards on Life Cycle Assessment (LCA) [ISO 14040 [ISO 14040: 2006] and ISO 14044].
IT	Information technology	

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Abbreviation	Term	Definition
kg	Kilogram	
kWh	Kilowatt-hour	
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 1440: 2006].
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].
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].
NACE	Nomenclature of Economic Activities	NACE (Nomenclature of Economic Activities) is the European statistical classification of economic activities. It is established by law.
NF_3	Nitrogen triflouride	See Greenhouse Gas definition.
N_2O	Nitrous oxide	See Greenhouse Gas definition.
OCF	Organizational Carbon Footprint	Carbon Footprint of an Organization.
	Primary data	Sometimes also called activity data. Data that concern processes inside the operational control of the company or data from specific processes in the product life cycle. A partial PCF 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, 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).
PCR	Product Category Rules	Set of specific rules, requirements, and guidelines for developing Type III environmental declarations for one or more product categories. [ISO 14025:2006]
	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]
	Removal	The sequestration or absorption of GHG emissions from the atmosphere, which most typically occurs when CO_2 is absorbed by biogenic materials during photosynthesis.
	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]

Abbreviation	Term	Definition
PFCs	Perfluorocarbons	See Greenhouse Gas definition.
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.
PRODCOM	Production Communautaire (Community Production)	See table 4.1
SF_6	Sulphur hexafluoride	See Greenhouse Gas definition.
SIC	Standard Industrial Classification	The Standard Industrial Classification (SIC) is a four-digit classification system that classifies industries according to business activities.
SMILES	Simplified Molecular Input Line Entry System	See table 4.2
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.
	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.
TÜV	Technischer Überwachungsverein (engl.: MOT)	
	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]
UNSPSC	United Nations Standard Products and Services Code	See table 4.2
	Utilities	The term "utilities" includes here: Electricity, process steam, excess steam, cooling water, demineralized water, process water, compressed air and nitrogen.
	Validation	the process of evaluating a system or component to ensure compliance with the functional, performance and interface requirements. [ISO/IEC 14776: 2010]
VAT	Value Added Tax	
	Verification	Confirmation, through the provision of objective evidence, that specified requirements have been fulfilled. [ISO 9000: 2005; ISO 14025:2006]
	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]
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.

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Appendix

Proposals for calculating proxies in the case of no primary or secondary data are available

Example: Landfill

The carbon content of the waste material shall be converted fully to CO_2e when waste is disposed of on surface landfills.

There shall be no GHG emissions allocation for waste that is disposed of in underground landfills or similar (e.g. deep well injection).

- Waste to underground landfill: no GHG emissions to be allocated.
- Waste to surface landfill: 100% conversion to CO_2e based on carbon content.

[BASF SE (2021)]

Example: Wastewater treatment

Emissions from treatment of wastewater that is generated during the production of a product A be allocated to the PCF of the product A.

The GHG emissions calculation from wastewater treatment shall include the emissions coming from the biological degradation as well as the emissions from the operation of the wastewater treatment plant and the disposal of the sludge (incineration etc.). The carbon content of the waste material shall be converted fully to CO_2e. As a basis for this calculation, the Total Organic Carbon (TOC) load of the process can be used if available.

If the Total Organic Carbon (TOC) load of your processes is known:

- 100% conversion to CO_2e based on carbon content.
- Utilities for treatment of wastewater and sludge incineration included using an emission factor of the treatment plant, e.g. 1 kg CO_2e from treatment of 100 kg waste water.

[BASF SE (2021)]

e.g. A product generates 100 kg wastewater per kg of product. The amount of product therein is 0.1 kg.

0.001 kg CO_2e/ kg waste water from electricity

0.0005 kg CO_2e/ kg waste water from sludge incineration

$PCF_{Product\ A}$ = 0.001 kg CO_2e/kg WWT electricity * 100 kg + 0.0005 kg CO_2e/kg WWT sludge incineration * 100 kg + 0.7 kg CO_2e/kg WWT TOC = 0.85 kg CO_2e/kg

Further information can be found at:

Hernández-Chover, V.; Bellver-Domingo, A., Hernández-Sancho, F.; (2018), Efficiency of wastewater treatment facilities: The influence of scale economies, Journal of Environmental Management, Volume 228, 77-84, ISSN 0301-4797, https://doi.org/10.1016/j.jenvman.2018.09.014.

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Overview examples of different allocation approaches

CO_2 emissions from Input kg/kg	Output materials	Amounts in kg	Amounts in mol	N content in kg N/kg	Prices in Euro/kg
5.00	Product A	0.2	0.3	0.1	20
	Product B	0.4	0.5	0.2	5
	Product C	0.3	0.2	0.3	1
	Total	**0.9**			

Mass allocation	Mass in kg outcome	Allocation factor: Mass / Total mass	Allocation factor * emission (B*5)	kg CO_2 per kg of product (C / B)
Product A	0.20	0.22	1.11	5.00
Product B	0.40	0.44	2.22	5.00
Product C	0.30	0.33	1.67	5.00
Total	**0.90**	**1.00**	**5.00**	

Economic allocation	Proceeds: Amount * Price in kg * Euro	Allocation factor: Proceeds / Total proceeds	kg CO_2 per kg of product (B * 5)
Product A	4.00	0.63	3.17
Product B	2.00	0.32	1.59
Product C	0.30	0.05	0.24
Total	**6.3**		**5.00**

Nitrogen content allocation	Proceeds: Amount * N in kg	Allocation factor: Proceeds / Total proceeds	kg CO_2 per kg of product (B * 5)
Product A	0.02	0.11	0.53
Product B	0.08	0.42	2.11
Product C	0.09	0.47	2.37
Total	**0.19**		**5.00**

Stoichio-metric allocation	Proceeds: Amount * mol	Allocation factor: Proceeds / Total proceeds	kg CO_2 per kg of product (B * 5)
Product A	0.06	0.19	0.94
Product B	0.20	0.63	3.13
Product C	0.06	0.19	0.94
Total	**0.32**		**5.00**

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tfs-initiative.com/scope-3-ghg-emissions