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 2.0 - November 2022

The full PCF Guideline has been launched by TfS

The first version of the PCF Guideline was published in September 2022, focusing exclusively on chapter 5 of the Guideline, prescribing in detail the specifications for supplier product carbon footprint (PCF) calculations within the chemical industry. The November 2022 release[1] launches the full open-source PCF Guideline for calculating PCFs and Corporate Scope 3 Category 1 (Scope 3.1) greenhouse gas (GHG) emissions. Four additional chapters complete the PCF Guideline, providing further insights about the guidance, reporting principles, and the major addition of guidance for Scope 3.1 calculation at corporate level.

Across the chemical industry, there is an urgent need to decarbonize – especially in the upstream value chain, beyond a corporation's own operations. Currently, a major share of the industry's greenhouse gas (GHG) emissions arises from the upstream value chain (scope 3). 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 new TfS PCF Guideline is unique in that it draws on the wealth of expertise and knowledge within the TfS member network to set a standard for the chemical industry, while remaining fully compliant with existing standards 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 suppliers 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 their own corporate inventories on the basis of supplier-specific data, while at the same time providing guidance on how to calculate the PCFs of their own chemical products, with the aim to create transparency and decarbonize the entire value chain. The PCF calculated based on the guideline will support downstream users for their calculations as well.

(1) In addition to the publication of Chapters 1-4, the following sections in Chapter 5 have been amended in this version: 5.2.9 – Multi-output processes, 5.2.10.4 – Carbon capture and storage & Carbon capture and utilization, 5.2.11.2 – Data quality rating, and 5.3.2 – Information to be reported with PCF.
No further amendments will be made to the PCF Guideline until the release of a new issue in accordance with the governance process outlined in Chapter 2.2.

01 Introduction

Anthropogenic greenhouse gas (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 greenhouse gas emissions and thereby must play an important role in reducing GHG emissions. 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 in order to prepare for potential future regulations. Particular attention should be paid to the Scope 3 category 1 (3.1) "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 their 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. 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 category1) represent a major share of many chemical company's greenhouse gas emissions. The TfS PCF Guideline enables corporations to account for Scope 3 category 1 GHG emissions in a systematic and meaningful way.

(1) https://www.weforum.org/agenda/2020/01/how-to-build-a-more-climate-friendly-chemical-industry/

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 PCF to 3.1 accounting is a harmonized approach that shows how PCF 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.

This guideline aims to provide instructions for the calculation and implementation to the subsequent reporting of 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 the 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 Guidance

2.1 Background and context

The global chemical sector initiative, Together for Sustainability (TfS), launches with this document the new 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.

The TfS initiative developed this guidance 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. [WBCSD (2013)]

2.2 Governance process for periodic review of the present guideline

This document is to be understood as a first version 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 guidance 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 guidance documents.

2.3 Problem statement

General problems described in chapter 2.1 are to be dealt with and described in more detail here. Relevance analysis of gaps in standards. 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 Product Carbon Footprint (PCF) calculation.

2.4.2 Embedding supplier PCF data in downstream PCF calculations calculation

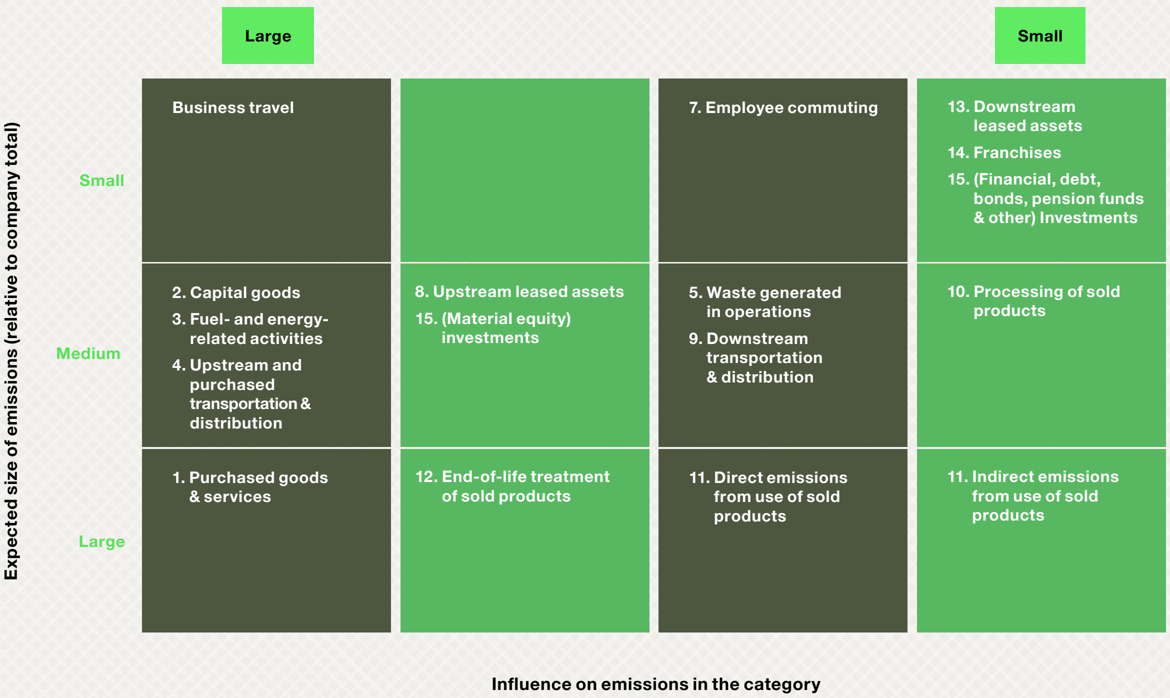
The application of chemicals is an additional topic and is covered in some specific GHG Protocol categories. PCF figures of high quality are needed to calculate meaningful cradle-to-grave applications. The guideline supports indirectly the reporting in these categories but is not in focus here. However, using recycling materials or bio-based materials from downstream applications as raw materials for chemicals are considered here as well, but are special topics where future guidance for an accurate reporting is needed. Probably the exiting categories must be adopted accordingly. TfS will work on these topics in future 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 guidance is given to increase transparency and increase harmonization in the sector. This guidance 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 2.3). For this reason, TfS decided to put the first focus of this guidance 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 chemicals, 2013)



The second part of this guidance focuses on specifications for embedding supplier PCF data into downstream customer's PCF calculations. As chemical products often are subjected to further processing, PCFs are vital to assess the contribution of the chemical industry on the environmental impact of other products (downstream: Scope 3.1).

Both the standardized methods for Scope 3.1 inventory and for PCF calculations will help chemical companies and their customers to credibly communicate potential impacts of their emissions 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 14064 -2: 2019
- ISO 14064 -3: 2019
- ISO 14067: 2019
- ISO 14040: 2006
- ISO 14044: 2006

The guidance 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 guidance 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 (2021), 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 guidance 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]

(1) https://www.iso.org/foreword-supplementary-information.html

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. 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.

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_2-eq 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_2-eq emissions result from the generation of purchased energy, such as electricity and steam used to power the reporting company's plants.

Scope 3 CO_2-eq 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 annual 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. Other Scope 3 categories are not considered herein unless there are interactions with category 3.1 that may result in inadequate calculation of total emissions if related aspects are not considered.

For chemical companies, the most emissions-intense purchased goods are often raw materials used and transformed to products. For annual corporate reporting, the PCF 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. This resulting PCF is the 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 in the reporting year. 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.
- 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 the supplier should be as close as possible to the time interval of the reporting company.
- 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.
- The attributes delivered with the PCF of the product. should be complete and representative for the product the purchased number and amounts of materials are available to calculate a correct mass balanced figure.

4.2 Foundations of the 3.1 accounting process

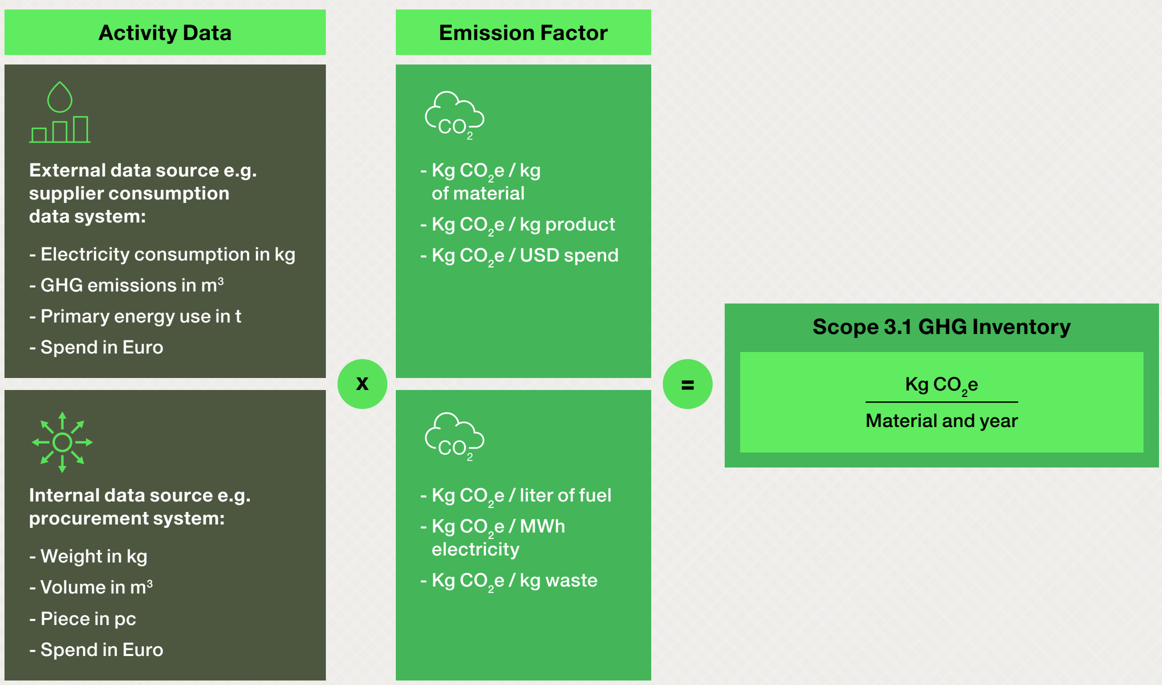
This section covers the best practices for building a GHG inventory and GHG emissions calculation techniques. A GHG inventory accounts for all GHGs emitted to or removed from the atmosphere by the reporting company. The GHG inventory will list, by source or GHG Scopes, the amount of GHG emissions emitted 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. 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 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.

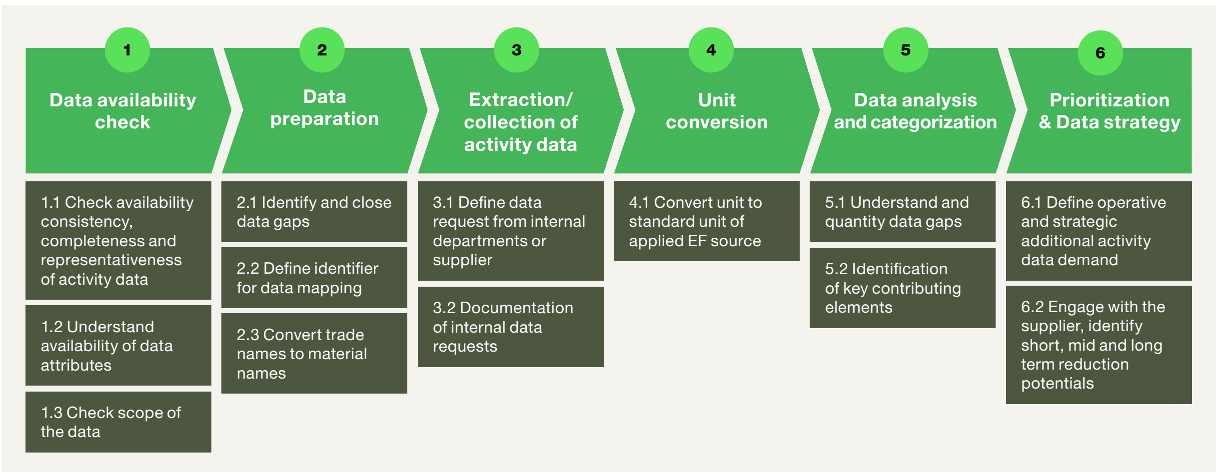
Data availability check

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

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



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.

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 often 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 4.2, 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 than 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 greenhouse gas 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 good 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) 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 Overview of impacts to Scope 3.1 reporting of different raw materials according to their share of contribution

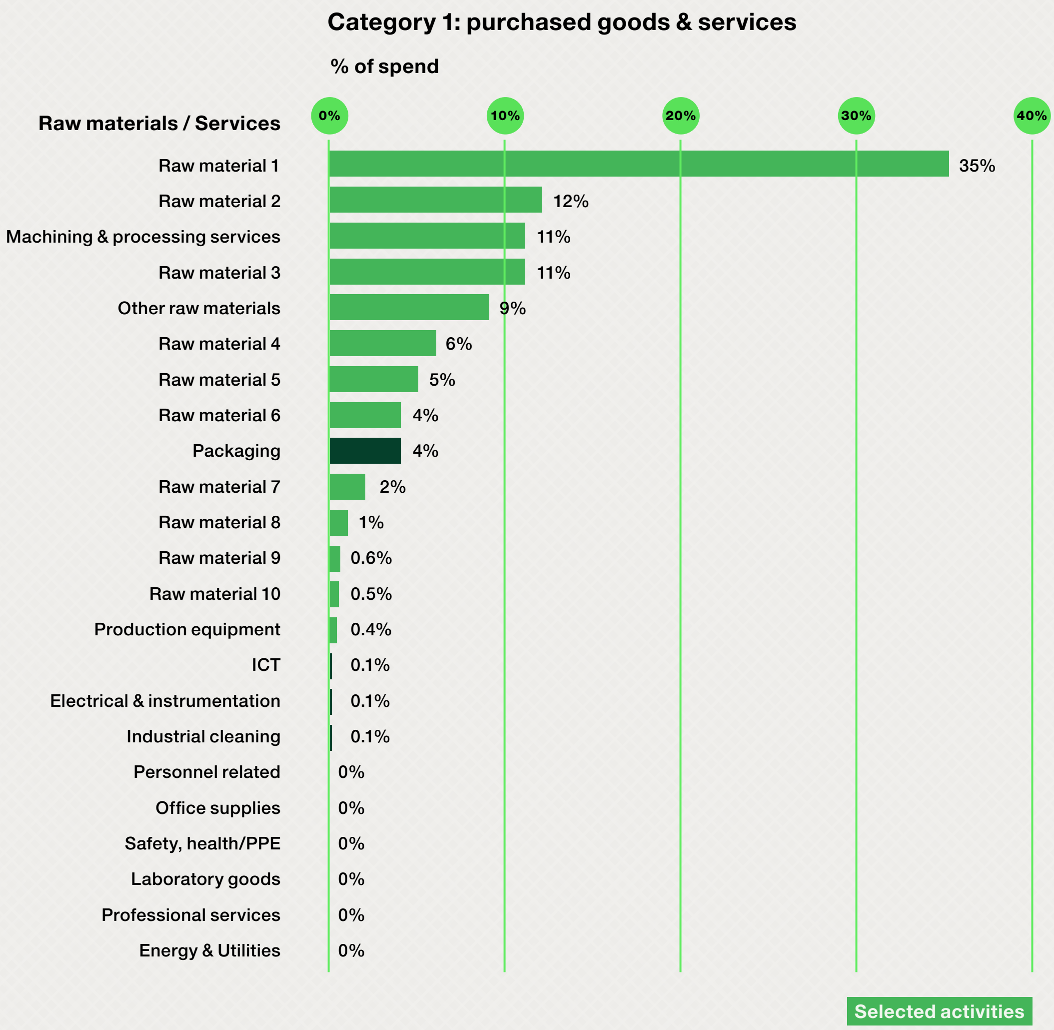


Table 4.2 Prioritization of goods and services based on CO_2 vs spend. Following the 80/20 rule, using top 80% of CO_2 emissions prioritizes only raw materials, whereas using 80% of spend prioritizes both raw materials and services.

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 a company case study below).

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 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 chemical company applied an emissions and spend-based analysis to prioritize its purchased goods and services before collecting data for category 1. The company set out to identify the purchased goods and services that collectively accounted for at least 80% of emissions as well as 80% of the total spend. The table illustrates how the prioritization results vary if consider GHGs vs spend; most notably, the inclusion of high-spend purchased services when spend is considered.

4.3.3 Activity data updates & improvement

Each year, the reporting company shall update the amounts of goods and services purchased. The company shall also account for any new categories and types of purchases. Any material errors identified that which 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 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 baseline, in order to maintain consistent comparisons.

4.4 Emissions 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 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 emissions factors (Figure 4.4).

1) Data availability check and emissions factor strategy

Emissions factor data 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 varified databases. Examples of emission factors sources are as follows:

- Verified data from associations such as ISOPA, Plastics Europe, Fertilizer Europe, World Steel association, etc.
- LCA databases such as GaBi (Sphera), 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), GREET, etc.
- Supplier data.

Companies should the check validity of the PCF by consulting the attribution list within chapter 5.3.

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 and steer their Scope 3 target (1.2). Guidance for such an emission factor prioritization is provided with the decision tree provided 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 (1.3). 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 4.2.

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

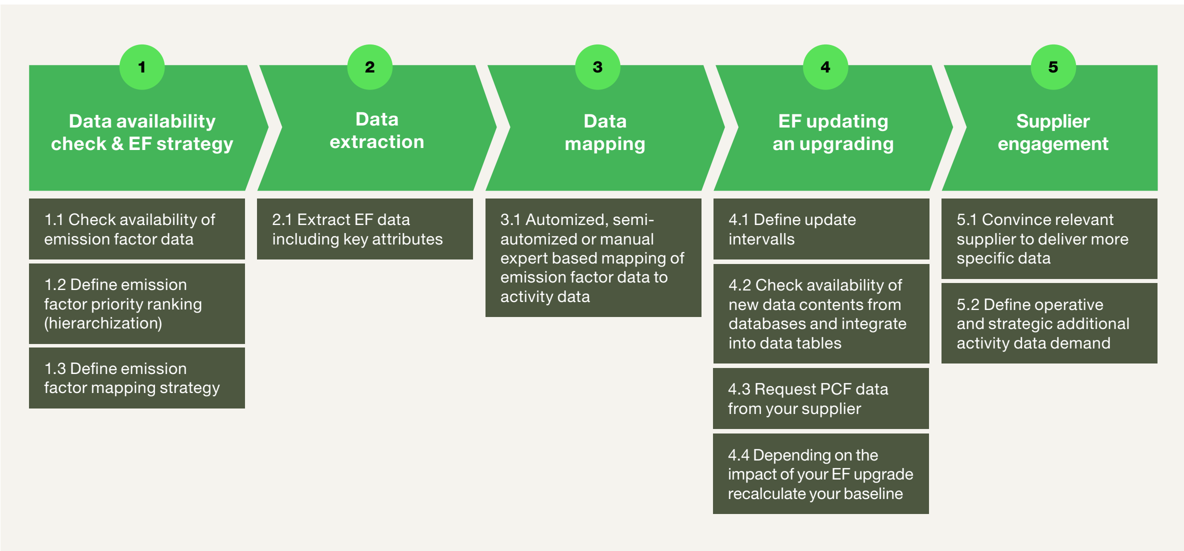


Table 4.3 Overview of data sources available for an accounting of emissions from Scope 3.1

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	Reporting company's procurement or ERP system
Source Emission Factors	Environmen-tally 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
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

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 factor data 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 chapter 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 4.4.

Table 4.4 Overview of data sources available for an accounting of emissions from Scope 3.1

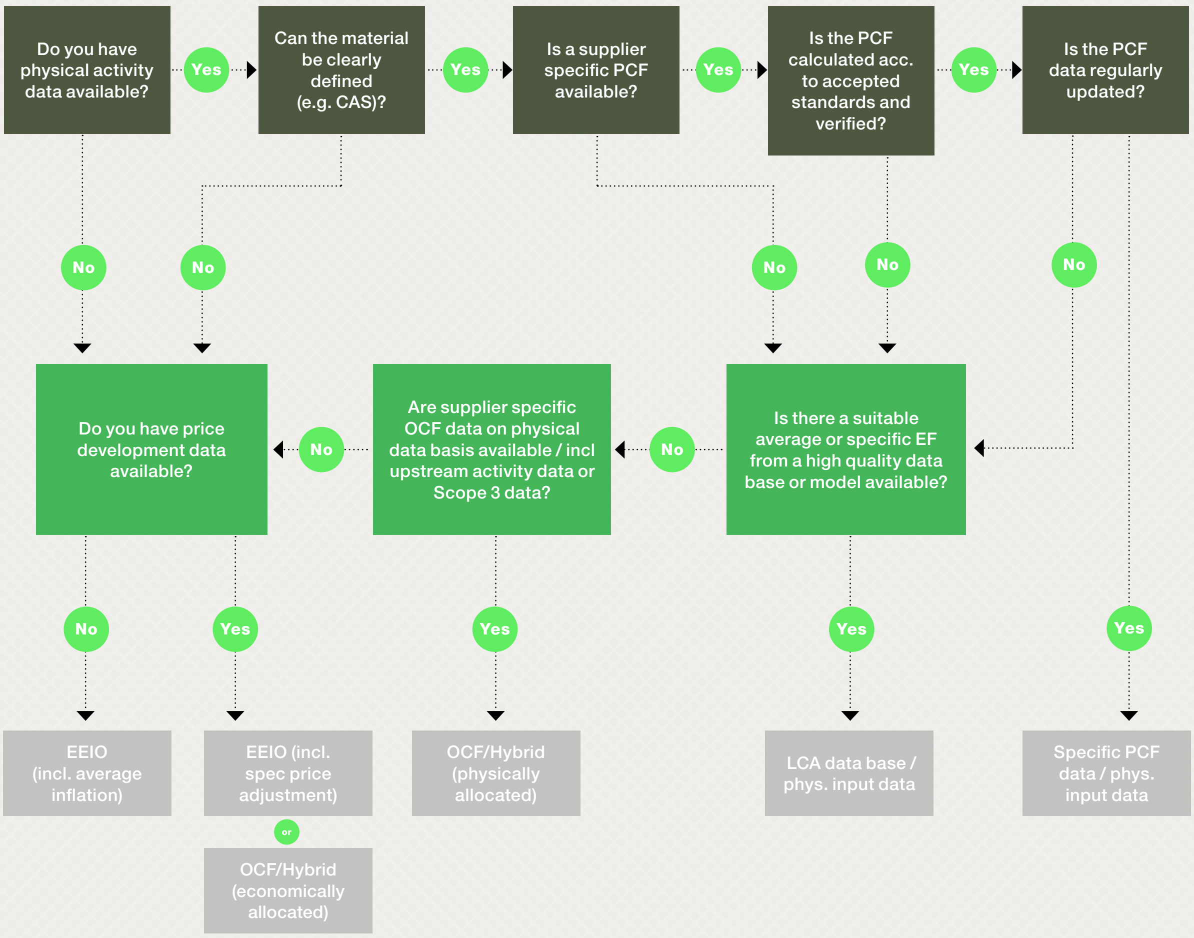
Estimation approaches	Application	Examples
Applying more accurate data/calculations for large contributors	If possible, apply a 80:20 approach	Collect primary data from your supplier for 20% of your purchased products that contribute 80% to the reporting companies Scope 3.1 footprint
Applying less accurate 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., 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 factor data 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. 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 TFS initiative WS 5.2). 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 appendix of this document. A decision tree supporting the decision process is shown in Figure 4.5.

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



4) Emissions factor updating and upgrading

If manually done, the attribution of emission factor data 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 (4.1). 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. 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 4.3). 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 align the baseline year 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 the more supplier specific methods, 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 total.
- 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 baseline year 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 (5.1). 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 help both parties to understand emissions driver of upstream but also product use and disposal better, it can also help to reduce concerns regarding the exchange of PCF data. Finally, an operative and strategic emission factor demand should be defined in the data management plan aligned with the reporting companies GHG reduction ambitions (5.2).

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 Us$ revenue) for relevant goods and services

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

4.5 Target baseline and recalculation

When companies choose to track performance or set a reduction target, companies shall:

- Choose a scope 3 base year and specify their reasons for choosing that particular year;
- Develop a base year emissions recalculation policy that articulates the basis for any recalculations; and
- Recalculate base year emissions when significant changes in the company structure or inventory methodology occur.

Recalculating base year emissions

To consistently track Scope 3 emissions over time, companies shall recalculate base year emissions when significant changes in company structure or inventory methodology occur. In such cases, recalculating base year emissions is necessary to maintain consistency and enable meaningful comparisons of the inventory over time. Companies are required to recalculate base year emissions when the following changes occur and have a significant impact on the inventory:

- Structural changes in the reporting organization, such as mergers, acquisitions, divestments, outsourcing, and insourcing.
- Changes in calculation methodologies, improvements in data accuracy, or discovery of significant errors.
- Changes in the categories or activities included in the Scope 3 inventory.

In such cases, recalculating base year emissions is necessary to ensure the consistency and relevance of the reported GHG emissions data. Companies shall recalculate base year emissions for both GHG emissions increases and decreases. Significant changes result not only from single large changes, but also from several small changes that are cumulatively significant. As part of the base year emissions recalculation policy, companies shall establish and disclose a significance threshold that is aligned the company's greenhouse gas ambitions. Companies shall apply the recalculation policy in a consistent manner.

The guiding principles for establishing recalculation policies and some additional topics for the chemical industry will be developed by TfS in a further independent document, a so-called white paper with proposals for the re-organization of reporting topics.
[GHG Protocol Corporate Value Chain (Scope 3) Standard]

4.6 Additional accounting and reporting guidance

In the chemical industry specific cases needs to be addressed because they cannot be covered by the commonly applied approach 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.

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 manufacturing goods using 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:

$$\text{Emissions}_{\text{Scope3.1}} = \text{Mass}_{\text{CMP}} * \text{PCF}_{\text{CMP}}$$

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 pre-cursors 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 anti-trust 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.

2) If the contract manufacturer can provide a full cradle-to-gate PCF, the reporting company which is the 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 CO_2e-intense raw materials), energies und utilities are provided by the client.

2) And it is assured that the contract manufacturer does not deploy any GHG-intensive 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 in 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. 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 non-essential 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 except for 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 acts additionally as a trader of materials, 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 the trading activity is a "trade on paper" (i.e., purchase and sale are carried out shortly one after the other) and not connected to any physical delivery or distribution of a material, the trading company may exclude the respective GHG emissions from its Scope 3 inventory. The reasoning behind this is that in these cases:

- Supplier-specific information is difficult or impossible to obtain because a long-term supply relationship normally does not exist and hence, the supply chain is not traceable.
- The frequent change of "owner" of the material and subsequent reporting of each owner would lead to a high level of double counting in Scope 3 emissions.
- The effort of data collection is s not justified for the purpose of this trade which is solely to achieve financial benefit.

[WBCSD (2013)]

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.

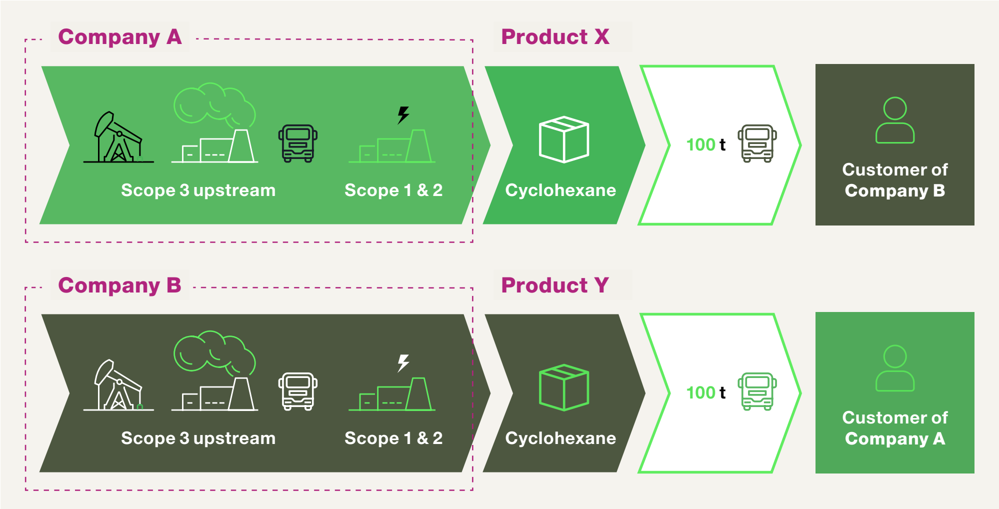
An example for a swapping agreement related to a chemical product is given as follows.

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 Scope 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). Example 2 is shown in Figure 4.6.

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



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).

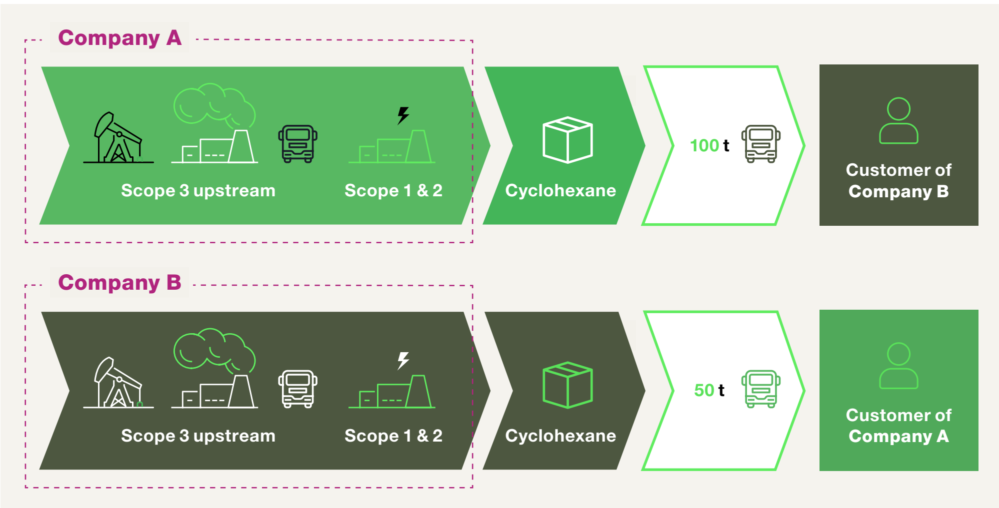
2. The Scope 3 emissions related to the transport of 100 tons of cyclohexane (Product Y) from the swapping partner (Company B) to its customer.

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 2 is shown in Figure 4.7.

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.

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)

The guiding principles for establishing recycled products and products with recycled content in the accounting for the chemical industry will be developed by TfS in a further independent document. In this document, the Chapters 5.2.8.4 gives guideline for calculating the PCF for mass balance calculations.

A waste is any residue of a production operation, transformation or use, any substance, material, product that its holder intends for disposal. Waste for final disposal has no economic value. The term secondary material is used for types of waste that can be used, recycled, re-used 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 S3.1 (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 4.5 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 + 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 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 will be developed by TfS in a further independent document. In this document, the Chapters 5.2.10.1 until 5.2.10.2 and 5.2.10.5 give guideline for calculating the PCF for biogenic removals and carbon.

4.6.6.1 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 Carbon uptake is balanced with the Carbon emissions in the EoL. ISO allows the calculation of the removal of biogenic Carbon and requests a separate emissions calculation depending on the application, the time frame of using the carbon etc. Long term uses or other ureses 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_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]. 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. 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)].

In 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 removals (e.g. biological GHG sequestration) emissions (mandatory).
- Separately: Any biogenic CO_2 removals e.g. biological CO_2 sequestration (mandatory).

4.6.7 Mass-balance chain-of-custody

The guiding principles for establishing biomass and mass balance products in the accounting for the chemical industry will be developed by TfS in a further independent document. In this document, the Chapters 5.2.10.5 gives guideline for calculating the PCF for mass balance calculations.

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]. 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 or other sustainable origin) 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. However, the content of the alternative raw material in the product is only attributed and, in most cases, cannot be traced by analytical methods e.g. C14-method for bio-based content.

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 book-keeping 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.

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 in 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.

4.6.8 Offsets, Carbon Capture and Storage (CCS) & Carbon Capture and Utilization (CCU) specifics

The guiding principles for products where offsets, CCU, CCS is applied in the accounting for the chemical industry will be developed by TfS in a further independent document. In this document, the Chapters 5.2.10.4 give guidelines for calculating the PCF for CCU and CCS.

Specific rules are applied for offsets, CCS, CCU. There is a direct or indirect removal included as one process step, very often out of the boundaries of the reporting company.

The guiding principles for products where offsets, CCU, CCS is applied in the accounting for the chemical industry will be developed by TfS in a further independent document. In this document, the Chapters 5.2.10.4 give guidelines for calculating the PCF for CCU and CCS.

In general, the following aspects shall be considered:

- The reporting company shall report all offsets separately from their Scope 1, 2 and 3 emissions. This includes both offsets with certificates and without.
- Any regulatory reporting requirements must be met.
- Following the guidance in the GHG Protocol Corporate Standard, companies shall report their emissions separately from offsets used to meet any GHG reduction targets that are established, rather than providing a net figure.
- Companies shall transparently mention the origin of reported offsets.
- Unbundled certificates shall be reported as separate offsets (i.e. do not adjust emission factors).
- Certificates that are purchased by the supplier of electricity (i.e. the supplier purchases certificates on your behalf) shall be reported as separate offsets.

- Emissions from purchased energy bundled to a Renewable Energy Certificate (REC) shall be reported based on the emission factor given in the REC. [GHG Protocol Scope 2 Guidance]
- 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)]

The organization may report optional information separately from the required information and the recommended information. Each type of optional information described below should be reported separately from the others.

The organization may report the results of contractual instruments for GHG attributes (market-based approach), expressed in GHG emissions (tCO_2e) as well as in the unit of transfer (e.g. kWh). The organization may report the amount purchased compared to the amount consumed.

The organization may report offsets or other types of carbon credits. If so, the organization:

- Shall disclose the GHG scheme under which they were generated;
- May add offsets or other types of carbon credits together if they originate from the same GHG scheme and are of appropriate vintage;
- Shall not add or subtract offsets or other types of carbon credits from the organization’s inventory of its direct or indirect emissions.

The organization may report GHGs stored in GHG reservoirs.

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, an attributes list and specific requirements were added to this document 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.

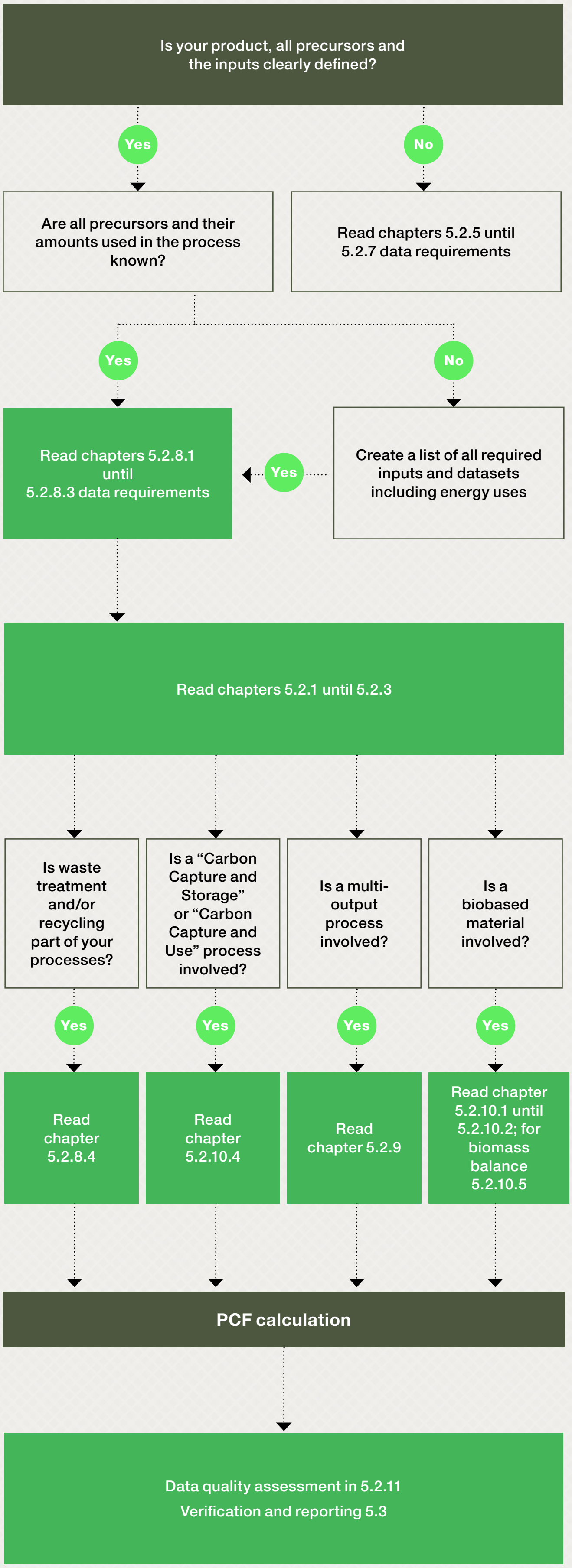
In Figure 5.1 an overview is given for easier navigation in the guideline document and to more easily find the most relevant chapters and skip others. Figure 5.1 should also give support for beginners in this topic to start relatively quick with the first calculations and follow-up with specific questions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

Currently, TÜV Rheinland Energy GmbH is providing the following services to TfS, which are expected to be completed in Q3/Q4 2022:

- Assess the guideline against all relevant standards applied (e.g. SBTi, WBCSD, GHG Protocol etc.).
- Check if reporting requirements for applicants are sufficiently defined in the guideline.
- Test the level of usability and giving hints for optimization.
- Loops of discussions and potential improvements during testing stage (WP 1-4 of TfS) and finalization stage (WP 1-5 of TfS).

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).

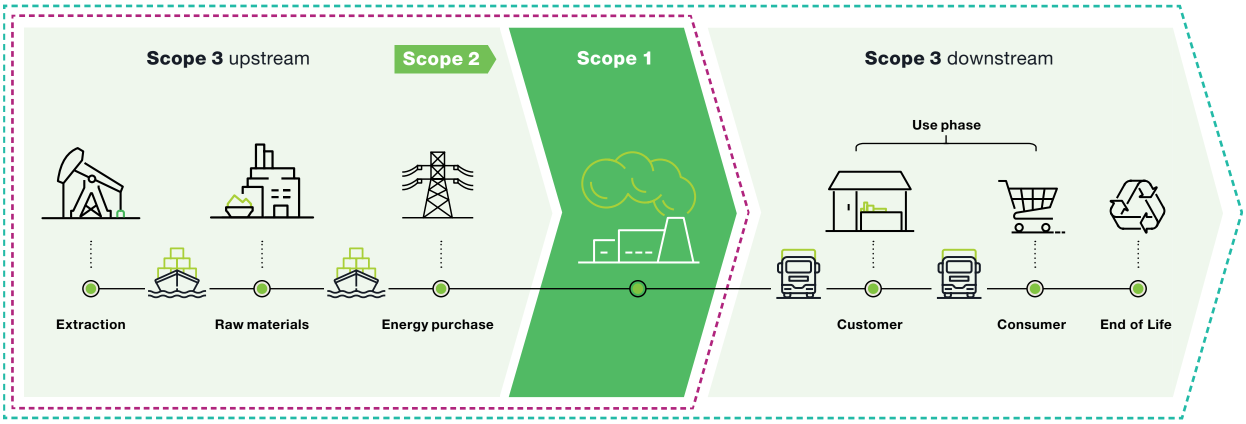
The guideline enables calculating the cradle-to-gate PCF based on standards and guidelines that were developed from different organizations.

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 and GHG Protocol. 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)].

Figure 5.2 System boundary definition



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.

As the guidance is product-related, the following activities are **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. [Pathfinder Framework (PACT powered by WBCSD)], Table 5.1. Please also see Chapter 5.2.3 on requirements to cut off activities.

The following activities might 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 might be included or excluded. For many chemicals, the contribution of packaging may be negligible within the context of a PCF in terms of mass and environmental significance. This is for example the case for bulk chemicals which are delivered by a supplier to customer manufacturing sites. For other chemicals, such as specialty chemicals or construction chemicals, packaging can play a more significant role in the PCF, namely for products sold in smaller units (e.g., in pails, cartridges, or wrapped rolls). In accordance with the cut-off criteria defined in section 5.2.3 of this guidance, packaging may be excluded or included in the PCF calculation, depending on its mass contribution and environmental significance. 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 describes generically the activities that shall be included or excluded from the system boundaries as well as the ones that are optional.

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 depending on the specific product and fulfilment of cutoff requirements
Utilities consumed	Business travel or employee commuting	Outbound transportation (if included in system boundary, it shall be stated separately)
Energy consumption	Production of investment goods	In-bound transportation if not relevant
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.

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), and in that case the PCF might be expressed per volume unit. In these cases, conversion factors (densities with associated conditions) shall be provided by the supplier for conversion to kg which is required in the attributes list in chapter 5.3. Any other unit of measurement like pieces or 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 pieces or 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 packaged product at factory gate.

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 [Pathfinder Framework (PACT powered by WBCSD)], [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 shall be as recent as practicable and **not older than five years**. The **most recent full year** (reporting- or calendar year) shall 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], [Pathfinder Framework (PACT powered by WBCSD)].
- **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, later 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 five 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 five years or if the production process has changed significantly, PCF values are no longer considered representative and must be re-calculated. According to EN 15804 [EN 15804 - 2: 2019], an EPD is valid for 5 years as well, after which it must be re-verified and typically revised. If no changes are detected after 5 years, the PCF value can be renewed by a statement as well. Once a PCF has been revised, the revised version will take over the original PCF and be valid for 5 years. However, we recommend initiating a review process for a PCF after 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.

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]. Making the initial identification of inputs based on mass contribution alone may result in important inputs being omitted from the study. Accordingly, energy and environmental significance should also be used as cut-off criteria in this process.

Requirements for PCF cut-off criteria

1. All material inputs that have a cumulative total of at least 95% of the total mass inputs to the unit process shall be included. But we recommend covering 98% or more to remove potential uncertainties and increase the level of completeness [BASF SE 2021].

2. All energy inputs that have a cumulative total of at least 95% 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, 98% of total energy inputs or more should be included.

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 that have a considerable upstream environmental footprint (e.g., precious metal like platinum group containing catalysts) should 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

This sectorial TfS 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. The work of the Partnership for Carbon Transparency's Pathfinder Framework (hosted by WBCSD) 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 Guideline**.

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

3. **TfS Guideline** if you do not have a PCR yet, the guideline can be used to calculate the PCF.

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

5. Pathfinder Framework (PACT powered by WBCSD); 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 different officially declared PCRs for the same product from different organizations exist, TfS will review them with an expert team and declare the "TfS accepted PCR". As a basis for the decision the correct application of the TfS guideline is first checked . TfS publishes and updates in every year 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.

Table 5.2 TfS accepted PCR (list can be adopted after review of PCR by TfS experts)

Product system	Standard/Rationale followed
Steam crackers	[Plastics Europe - Steam Cracker Allocation [2017]]
C12-14 Fatty alcohols (oleo), methyl esters, refined oils, and crude oils from oil palm, refined- and crude oils from Coconut	[ERASM 2014]
Toluene diisocyanate (TDI), Methylene diphenyl diisocyanate (MDI)	[ISOPA 2012]
Chlorine (chlor-alkali process)	[EUROCHLOR 2022]

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.

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.

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.

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

Table 5.3 Data hierarchy for energy and material inputs regarding primary, secondary and proxy data [Pathfinder Framework (PACT powered by WBCSD)]

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.

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. 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.

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.

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, Fertilizer Europe, World Steel association etc.
- LCA databases such as GaBi (Sphera), Ecoinvent, Carbon Minds, Agribalyse, ELCD (PEF), IDEA database, etc.
- Official national emission factor databases such as US EPA, IEA, Defra, GREET 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 of secondary data shall be specified in the report. The attributes list requirements in Chapter 5.3. describe in detail, which attributes 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 on 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:

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

Formula 1
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.

Specifications

The basic equation to calculate CO_2e for a direct emission is:

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

Formula 2
The types of emission factors needed depend on the types of activity data collected.

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	LIFE CYCLE INVENTORY (LCI) DATA	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	CO_2 0.2 kg CO_2e / kWh	CO_2 0.2 kg CO_2e / kWh	CO_2 0.2 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 for 120 km	CO_2 CH_4 0.2 kg CO_2 0.01 kg CH_4 / kWh	CO_2 CH_4 1 kg CO_2e / kg CO_2 + 30 kg CO_2e / kg CH_4	CO_2 0.5 kg CO_2e / kWh	CO_2 2.7 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	CO_2 2 kg CO_2 / kWh	CO_2 2 kg CO_2 / kWh	CO_2 2 kg CO_2e/ kWh	
List of activities within system boundary to produce the product	Different sources for emission factor data are available		Per declared unit 1 kWh	Inventory of GHG emissions per declared unit	GWP-factors translate individual GHG into the common unit CO_2e	Aggregated GHG emissions in CO_2e per declared unit	

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 Euro Chlor [EUROCHLOR 2022]. Proxy secondary data for the PCF of input materials were extracted from Winnipeg [Winnipeg CO_2 Emission Factors].

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	LIFE CYCLE INVENTORY (LCI) DATA	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 factor data are available		Per declared unit 1 kg Chlorine	Inventory of GHG emissions per declared unit	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), Nitrogen triflouride (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].

The 100-year GWP characterization factors according to the IPCC's Fifth Assessment Report (AR5), Appendix 8.A (Lifetimes, Radiative Efficiencies and Metric Values) may be used in 2022 during the transition period [IPCC 2013- The Physical Science].

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 should 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. These may be the same total where direct line transfers of energy are used [GHG Protocol Scope 2 Standard].

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 processes (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

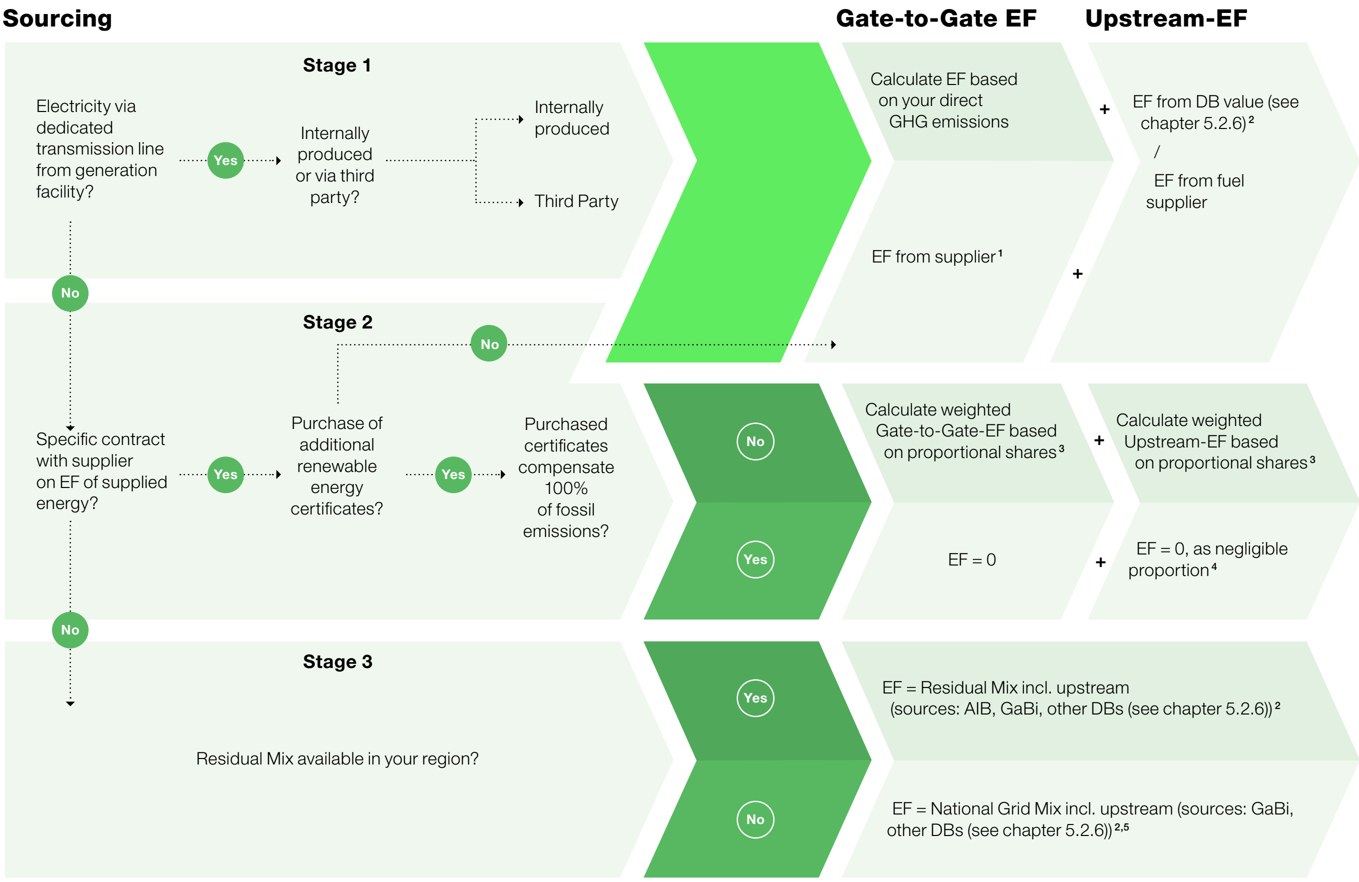
For the use in the PCF calculation organizations should generally calculate the emissions of electricity following the market-based approach (as described in the GHG Protocol Scope 2 Guidance). The electricity accounting approach used should be addressed in the PCF reporting. Please follow the decision tree in Figure 5.5 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 the three stages (which are additionally explained below in more detail):

- Stage 1: Electricity via a dedicated transmission line (market-based).
- Stage 2: Electricity from the grid (location-based) or specific contract with supplier on energy mix (market-based).
- Stage 3: Residual Mix (no specific contract with supplier on energy mix or no specific data available).

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 5.5).

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
$= EF_{Weighted} = 0.2 \times EF_{RE} + 0.8 \times 0.5 \times EF_{FE} + 0.8 \times 0.5 \times 0$).

(4) If impact lies within the cut-off range (s. chapter 5.2.3), apply EF = 0. Otherwise, please use DB value (GaBi or other DBs (see chapter 5.2.6)).

(5) Alternatively, IEA-Data can be implemented if additional Upstream-EFs from DBs (GaBi 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

Additional upstream GHG emissions (e. g. from mining and transport of fuels to the electricity generation facility) 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 and no further renewable energy attribute certificates are purchased, then the organization shall use GHG emissions from a supplier-specific electricity product.

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, then a proportional gate-to-gate 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, the gate-to-gate emission factor can be set to zero.

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) 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 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 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.

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

The same requirements and provisions for Renewable Electricity are applicable to other Renewable Energy forms, including Renewable 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. EXAMPLE: Contractual instruments can include energy attribute certificates, renewable energy certificates (RECs), guarantee of origin (GoOs) or green energy certificates.
- 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 Pathfinder Framework [Pathfinder Framework (PACT powered by WBCSD)], 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 Pathfinder Framework [Pathfinder Framework (PACT powered by WBCSD)], 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.

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).
- Only if the contribution to the overall PCF is significant (see chapter 5.2.3), in-bound transportation as e.g., transportation to an internal storage location as part of a company's direct activities should be considered.
- The transportation of an intermediate product from one production site to another shall be considered if relevant according to the cut-off criteria.

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.

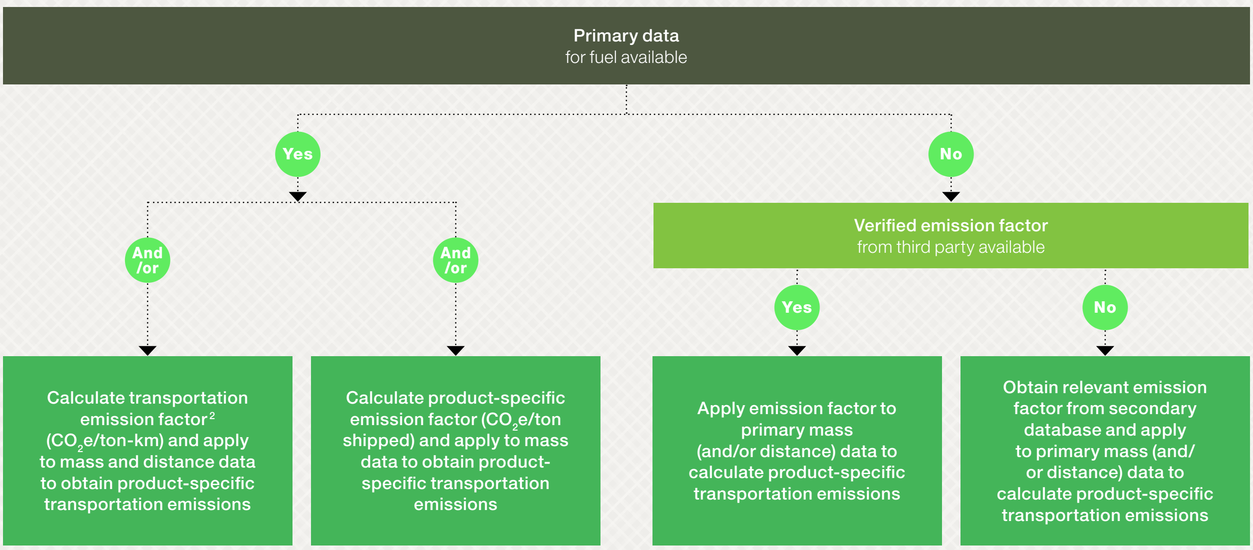
Transports can either be carried out directly by the reporting company e.g., in company-owned or leased vehicles, or by external transport service providers. As such, the method used to calculate product-related transport emissions is very much dependent on the availability of information such as fuel 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), [Pathfinder Framework (PACT powered by WBCSD)]. This guidance is not available anymore in the updated version of the 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 ton-km) 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 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.

Figure 5.6 Steps for calculating product transportation emissions [Pathfinder Framework (PACT powered by WBCSD)]



(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.

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 that is under development will give 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 substance or object which the holder discards or intends to discard per European Waste Framework Directive [EU Waste Framework Directive]. Waste has no economic value.

A co-product is a product that is produced in a multi-output process incidentally to the production of products that are intendedly produced and have the highest economic value in such a process[1]. Co-products have an economic value and 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.

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.

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

- 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.

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. Since waste is considered an output without economic value, no production emissions are allocated to the actual waste generated during production.

Typical waste treatment operations include disposal activities such as:

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

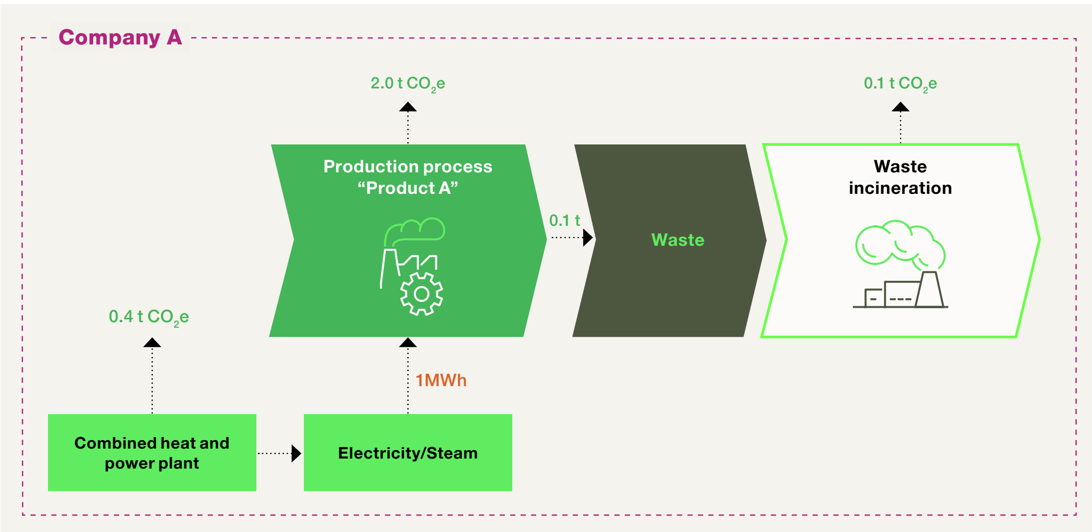
In some cases, different types of waste streams are co-treated in a single waste treatment facility, for example in the case of co-incineration of high and low calorific value waste streams or wastewater treatment for wastewater streams with different compositions. Such a waste treatment processes are multi-functional, 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).

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.

Figure 5.7 Waste incineration without energy recovery and without use of the energy



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

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 for material recycling can be found below.

Material recycling and waste treatment with energy recovery are considered separate and not equal. 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 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 5.4). 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.

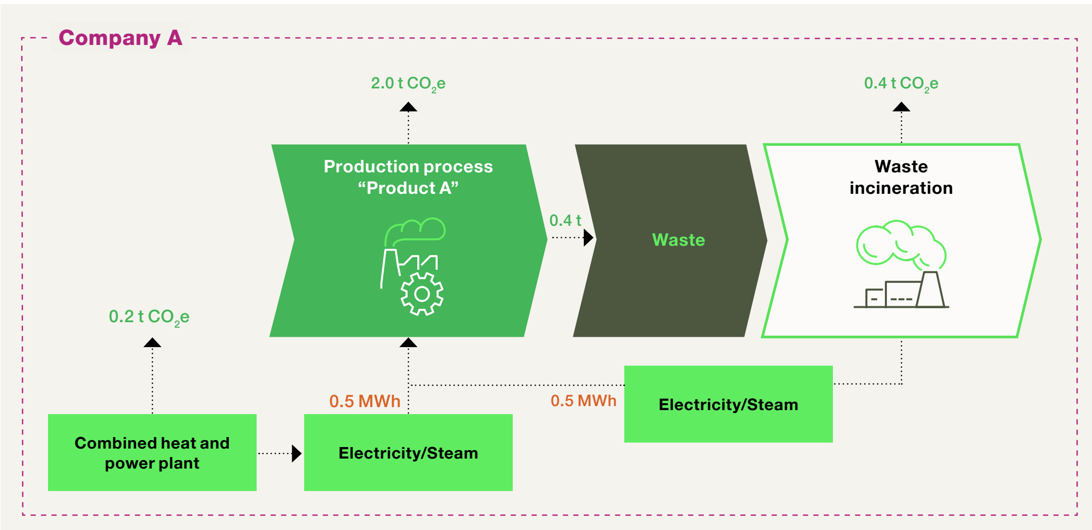
Energy recovery within the system boundaries of a product

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.

Figure 5.8 Waste incineration with energy recovery within the system boundaries of the company



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

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 5.4 Overview of different assessment approaches

	Cut-off approach 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 WBCSD Pathfinder + 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 GHG reporting	Corporate reporting has to be adjusted	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.

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".

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.

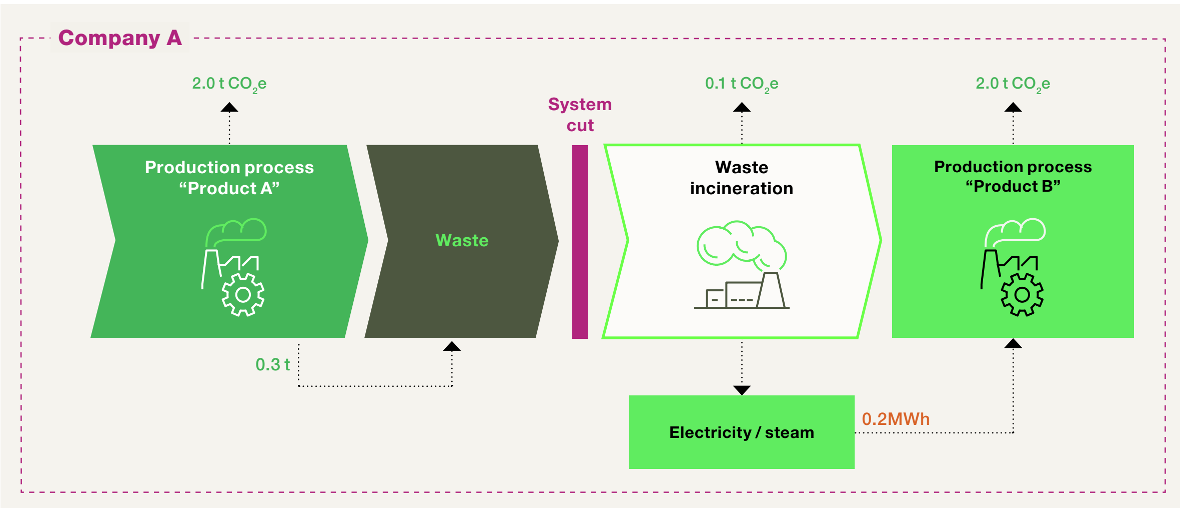
Following the cut-off approach, the impact of the waste treatment process shall be allocated to the user of the energy, product B. No impact from the production process for product A shall be allocated to the PCF of product B. If any of the processes, e.g. the production process "Product B" is not operated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

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.

Figure 5.9 Energy recovery from waste incineration with application of the cut-off approach



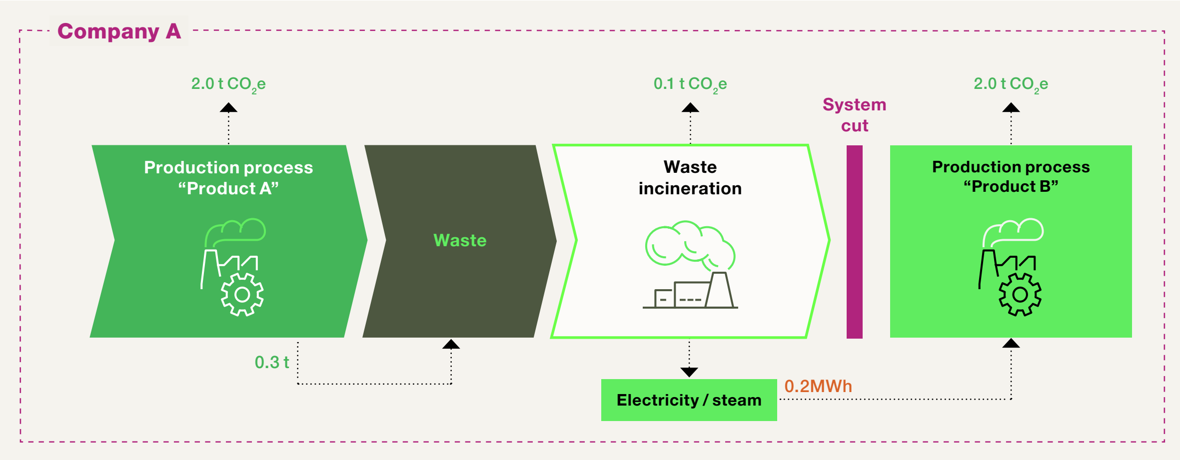
$PCF_{\text{Product A}} = 2.0\ t\ CO_2e / t$

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

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

Specifications

Figure 5.10 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:

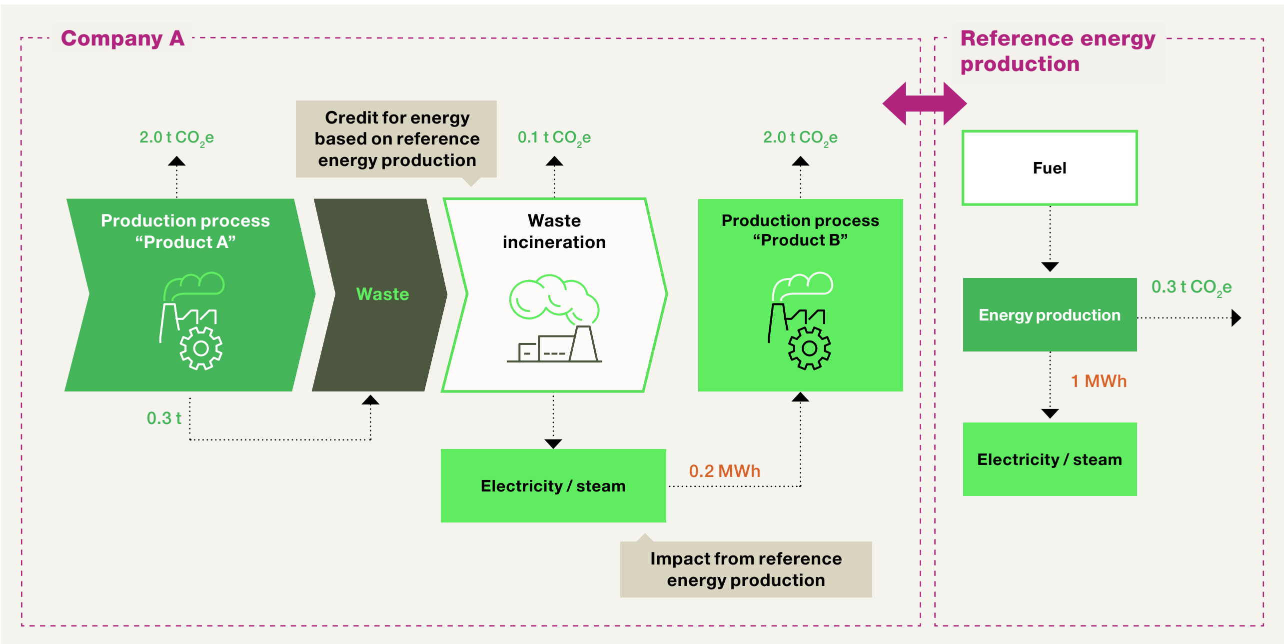
The substitution approach is a method to distribute the impacts of multifunctional process (e.g. waste treatment with energy recovery) between the waste generating and energy using system. Following the substitution approach this is achieved, with the help of including a reference system for energy production.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

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.

Figure 5.11 Energy recovery from waste incineration with application of the substitution approach



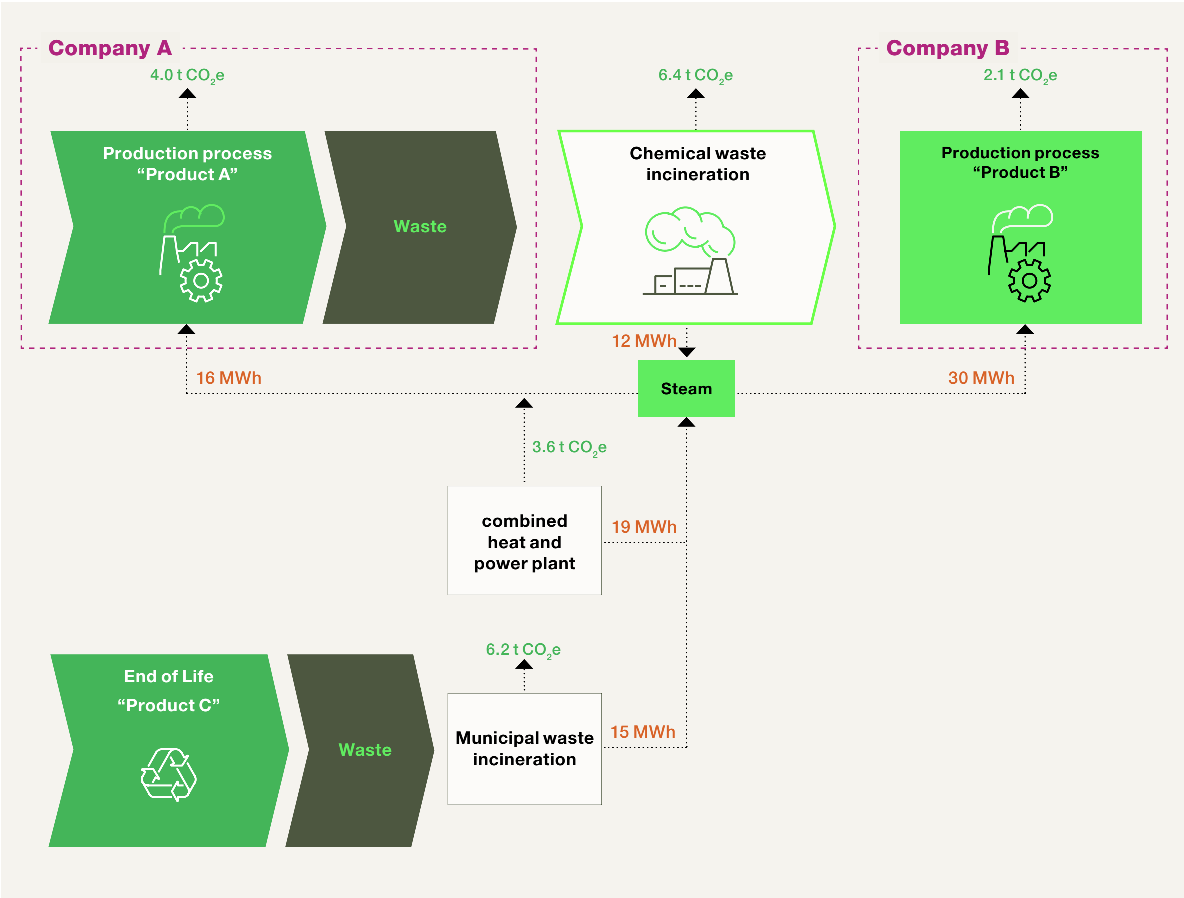
PCF $_{\text{Product A}}$ = 2.0 t CO_2e/ t + 0.1 t CO_2e/ t – 0.2 MWh * 0.3 t CO_2e /MWh = 2.04 t CO_2e/ t
PCF $_{\text{Product B}}$ = 2.0 t CO_2e/t + 0.2 MWh * 0.3 t CO_2e /MWh = 2.06 t CO_2e/ t
PCF $_{\text{Reference Energy}}$ = 0.3 t CO_2e/ 1 MWh

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. 1t of product A and 1t of Product B are produced in the system. 1t of product C is treated at its end of life.

Figure 5.12 Example of interlinked system with energy recovery from both production and municipal waste



Specifications

Table 5.5 PCF calculation for example of Figure 6 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 de-fossilize 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 existing standards, including the GHG Protocol.

The following section is focussing on the assessment of post-consumer waste recycling. Post-industrial waste streams of high quality and/or high value that will be recycled and therefore used in another application shall be assessed 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 are various types of mixed plastics waste after the sorting step and separating materials that cannot be handled in e.g., mechanical recycling. If a recycling technology enables waste to be used as a feedstock (and thus prevents other less favorable end-of-life options and keeps carbon in the loop), it creates societal benefits in 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" [Pathfinder Framework (PACT powered by WBCSD)].

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.

Both methods are explained in the following text providing 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.

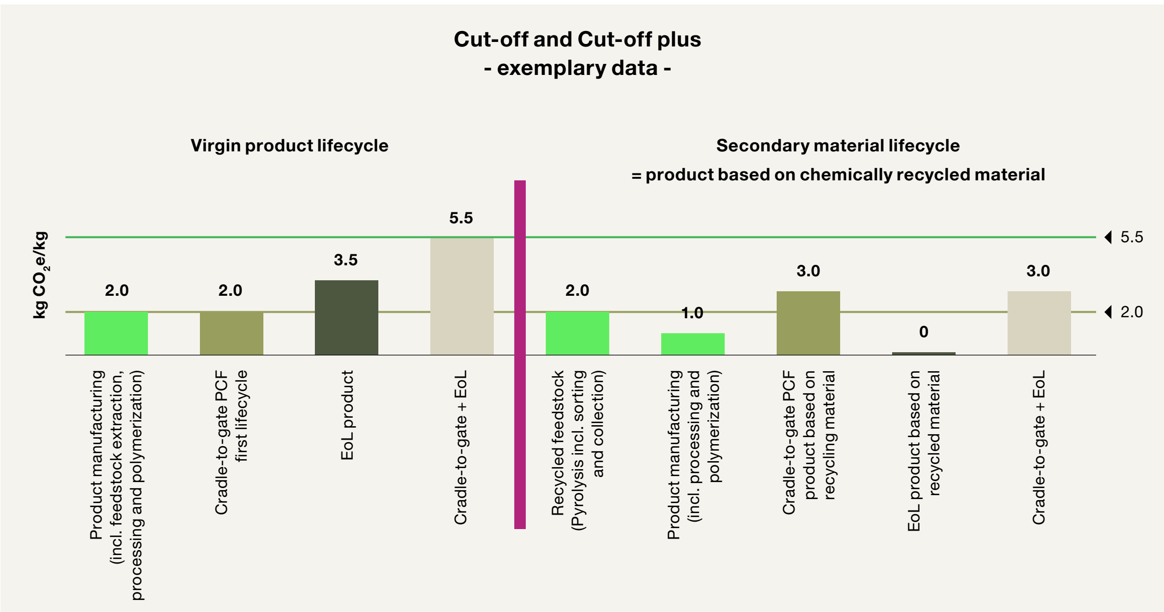
Example Cut-off and additional information

Standard reporting for cut off as follows:
PCF virgin (cradle-to-gate first life cycle) = 2.0 kg CO_2e /kg
PCF secondary material (cradle-to-gate first life cycle) = 3.0 kg CO_2e /kg

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

Specifications

Figure 5.13 Cut-off and additional information approach - exemplary data



The assumed EoL technology in this example 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 close to the cut-off approach described in the GHG Protocol. Through the additional information of the cut-off plus, the benefit of the recycled material compared to a virgin material becomes apparent.

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 relevant other available treatment methods.
- Being a new technology with 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, the requirements shall be clearly defined.
- ISO compliant substitution approach is applied, 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 deducted. As a basis for EoL impact estimations, the country mix of disposal technologies of the country of origin shall be considered if there are 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 the chemically recycled products results from the burdens of the recycling deducted by the savings of the counterfactual scenario, because the technology is benefiting to societal CO_2 savings by replacing the less favorable waste treatment option.

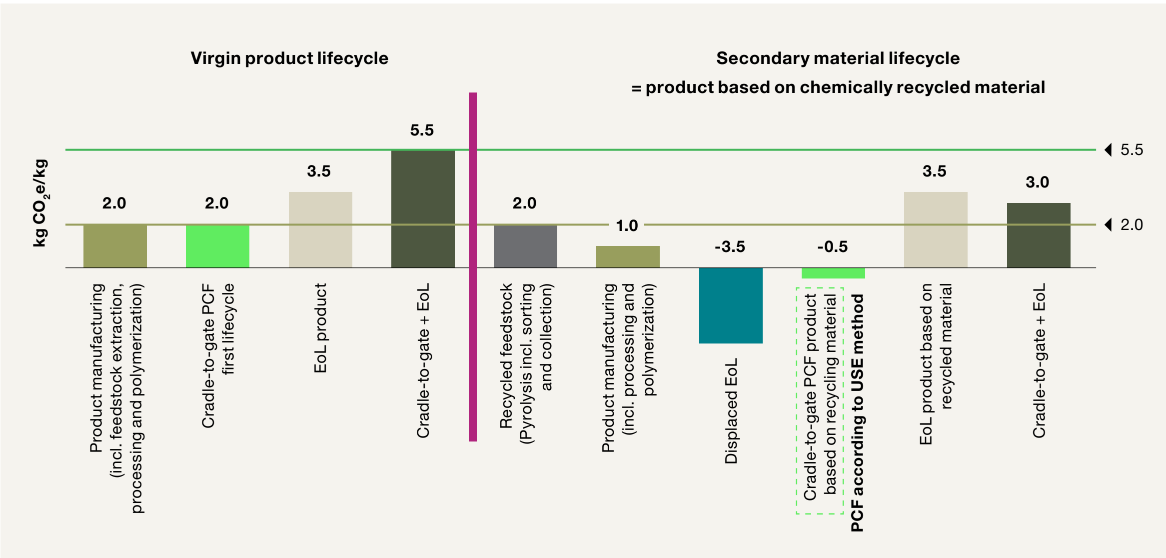
With this approach, benefits of the recycling of materials can be shown but are beyond a cradle-to-gate scope.

Example USE

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

Figure 5.14 USE approach - exemplary data



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

This approach is different to 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_2eq 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. Energy is in this sense understood as direct energy e.g., from exothermal reactions [Pathfinder Framework (PACT powered by WBCSD)]. Waste materials that go directly to a final disposal, e.g., an incineration or landfill, are not co-products as they do not have an economic value 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, the WBCSD Pathfinder Framework and the European Commission Environmental Footprint recommendations, the following steps shall be applied to attribute impacts in multi-output situations (see Figure 5.15):

1) 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 sub-metering specific process lines and/or using engineering models to model the process inputs and outputs [GHG Protocol Product Standard].

2) 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.

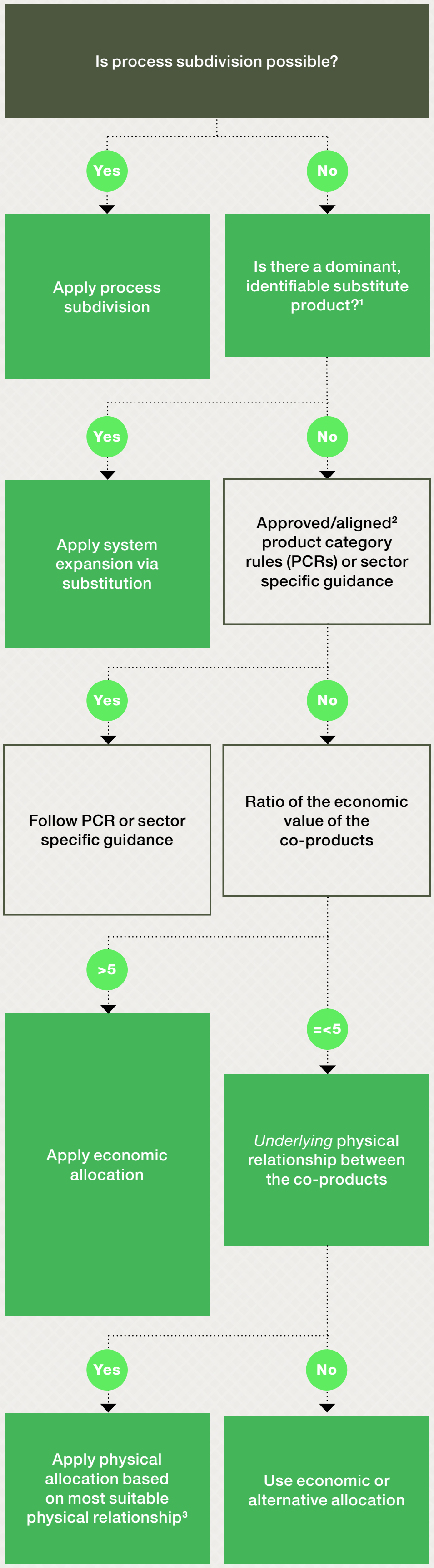
d. There is consensus for a production path of the displaced product agreed by TfS. Note: TfS will maintain and publish a positive list of processes and products.

3) The approach described in published and accepted product category rules (PCR) or Industry Association projects, 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.

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 will align with WBCSD and Catena X on the allocation hierarchy and thus the allocation approach as described in a PCR might be prioritized before System expansion and substitution. As already ranked very high, PCR will overrule other approaches.

Figure 5.15 Decision-making tree to show allocation rules and reduce assessment burden downstream [Pathfinder Framework (PACT powered by WBCSD)]



5.2.9.1 Substitution

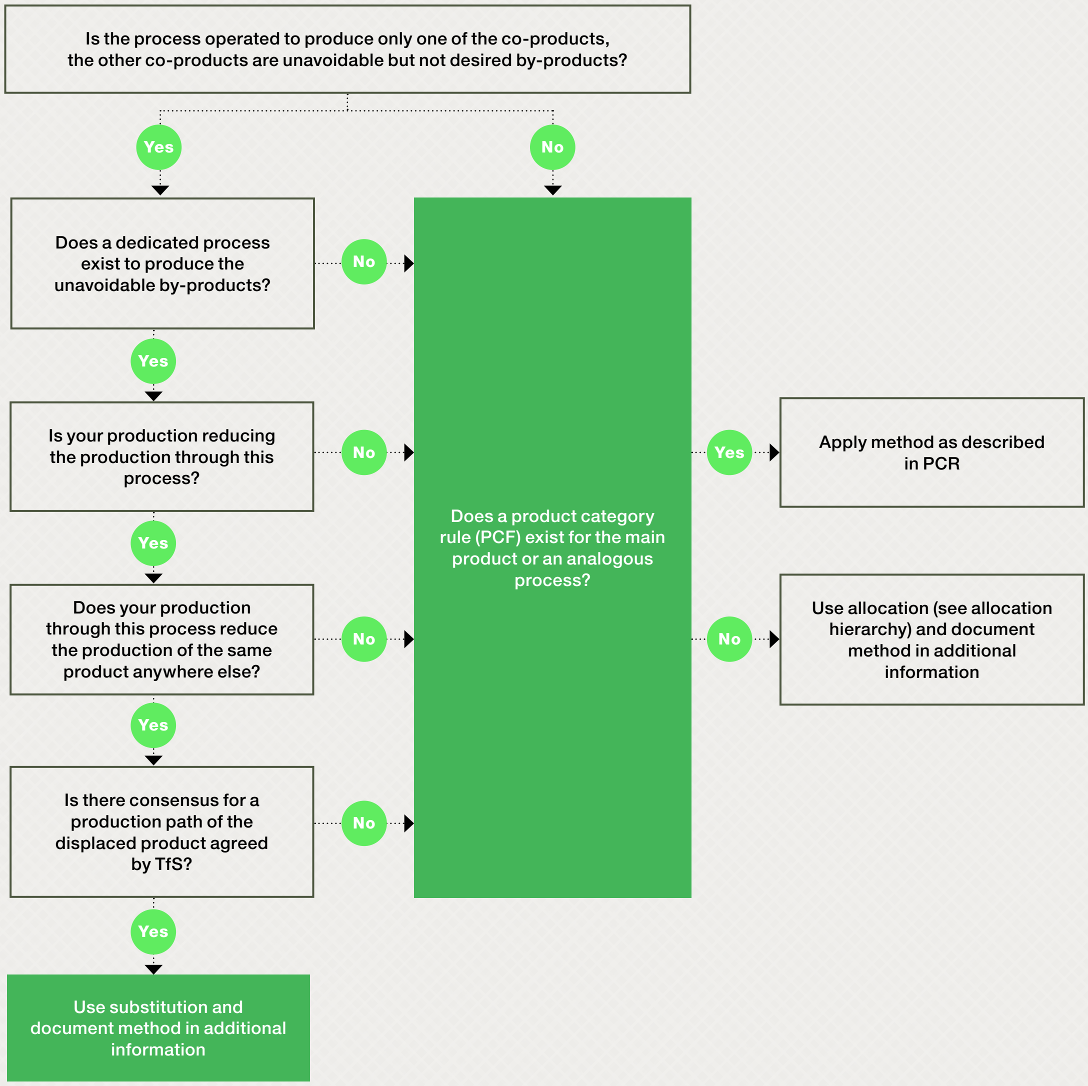
In Substitution, the co-products of process are compared to similar alternative products, and the environmental burdens associated with the alternative product(s) are subtracted from the product system under study to obtain the impact of the main product of the production process (see Figure 5.17) [ISO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

(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) 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.

(3) 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).

Figure 5.16 Decision tree for the application of substitution, PCR, and allocation



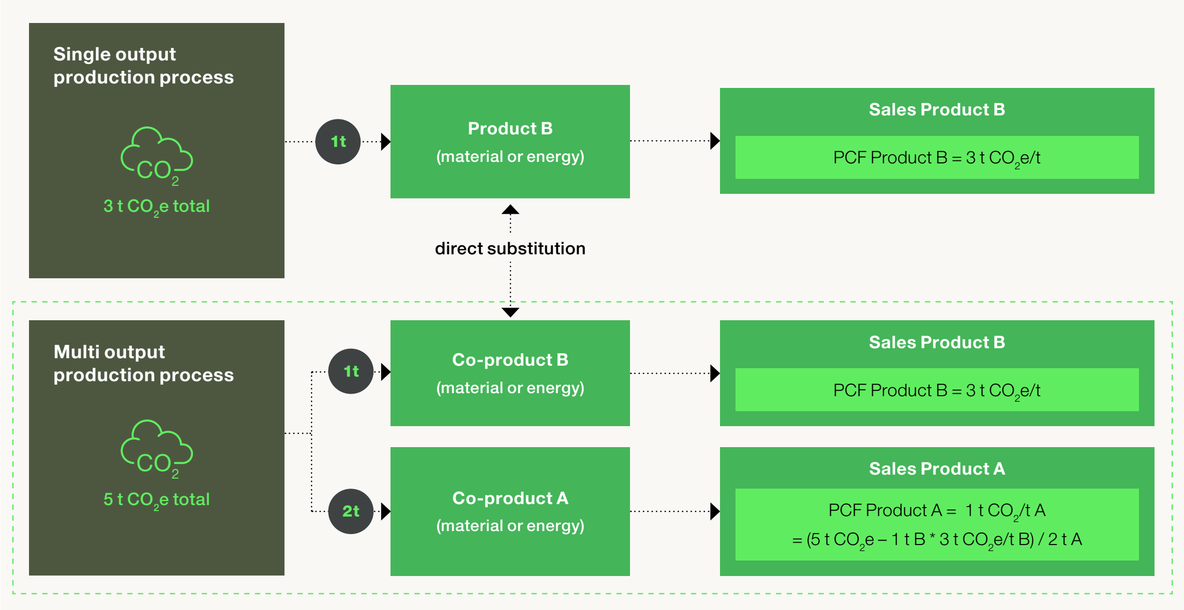
Specifications

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 5.16). Process subdivision is not possible, and a product category rule does not exist. The process is operated and optimized to produce co-product A as the main product. Co-product B is unavoidably co-produced and is considered a by-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 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 as e.g. 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 5.15. [Pathfinder Framework (PACT powered by WBCSD)]:

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). 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:

  a. Existing regional law.
  b. PCRs from world-wide operating associations.
  c. PCRs from regionally operating associations. (e.g., Plastics Europe).
  d. 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 the Pathfinder project and aligned with TfS (Figure 5.15). 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 market prices are not available, other economic factors 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 is be treated separately (see chapter 5.2.10.3 Carbon Capture & Utilization).

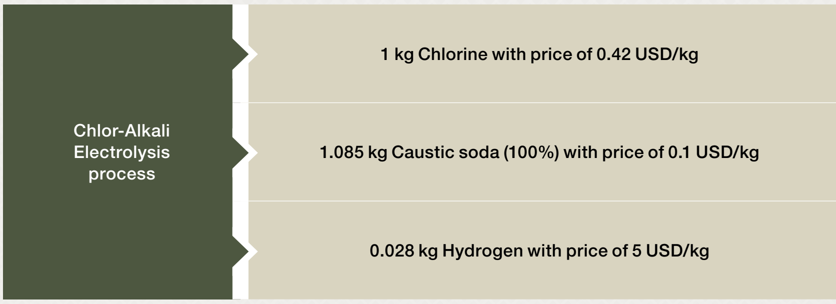
2. If hydrogen is a co-product allocation by heating value shall be applied because of the low molecular weight of hydrogen. Example: Syngas process that generates CO and hydrogen, both are gases and valuable products. If hydrogen is a co-product in a multi-output process, mass allocation shall not be 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 5.18). 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 5.18 Outputs of a Chlor-Alkali electrolysis process



It should be noted that an association document exists for the 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 5.6).

Table 5.6 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 would 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 5.7).

Table 5.7 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 5.8).

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.

Table 5.8 Example calculation for economic allocation

Definition	Value [USD/kg]	Mass [kg/kg Chlorine]	Value x Mass [USD]	Share of impact
Chlorine	0.42	1.00	0.42	63%
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.

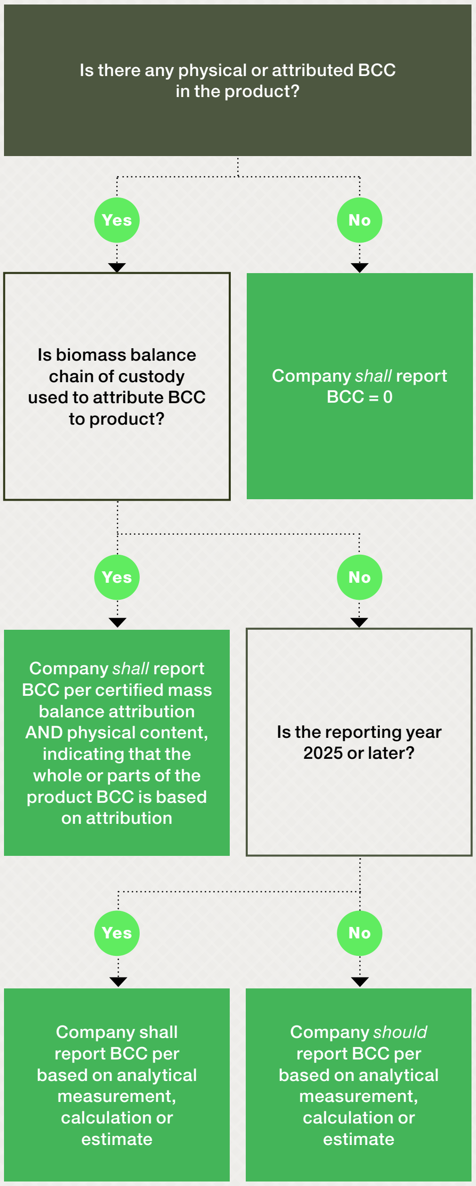
Overview of calculation examples with a multi-output-allocation

Table 5.9 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 is 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

Figure 5.19 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.

(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" [GHG Protocol Corporate Standard], 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". As biobased materials origin from plants, the same is true for them."

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].

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 as well and 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 in scope of this document [BASF SE (BASF)], [ISO 14067: 2018]. Figure 5.19 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]).

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 (carbon molecular weight / 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 emission[1]. If the ethanol is used as a pre-cursor 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 biobased ethanol is provided below in table 5.10.

Table 5.10 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)	0.521	0.521
Equivalent biogenic carbon removal in product, expressed in carbon dioxide (kg CO_2/kg ethanol)	-1.9	0.0
Equivalent biogenic carbon overall removal, expressed in carbon dioxide (kg CO_2/kg ethanol)	-2.334	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	0.1
Emissions, biogenic (kg CO_2e/kg ethanol)	0.8 (0.4 from Methane)	0.4 (Methane)
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	-2.334+0.2+0.8+2.0 = **0.67**	0.0+0.2+0.4+2.0 = **2.6**

(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).

- Biogenic methane emission and corresponding CO_2 uptake:
  0.4 kg CO_2e / kg ethanol

  0.4 / GWP factor methane (30 kg / kg Methane) = 0.013 kg Methane / kg Ethanol

  0.013 kg methane = (0.013/16) * 44 = 0.04 kg CO_2 uptake

- Additional uptake from biogenic CO_2 emission:
  0.4 kg CO_2e / kg ethanol
- Total CO_2 uptake:
  -1.9 kg CO_2 – 0.04 kg CO_2 – 0.4 kg CO_2 = -2.34 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: 0.5217 kg C / kg Ethanol.
- Total carbon content: 0.5217 kg C / kg Ethanol (= biogenic carbon content of 0.5217 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. The following requirements should apply for the usage of mass balance chain of custody in determination of PCF:

1. The biomass used should follow a transparent certification standard and the conformance to the certification should be verified by an independent and qualified independent party.

   a. The certification system shall have clear chain of custody rules, traceability requirements, defined boundaries, guidelines for marketing claims, include safeguards against double counting in any sense, and shall identify the type of sustainable raw material throughout the supply chain.

   b. Examples of acceptable certification systems include ISCC PLUS, REDcert2, UL ECVP 2809, RSB Advanced Materials, FSC, RSPO, or equivalent.

2. The LCA of the manufacturing process in which the mass balance attribution occurs can be reviewed by an independent party and confirmed to be in conformance with ISO 14044 [ISO 14044: 2006] or ISO 14067 [ISO 14067: 2018]. The study shall document how the material flow and attributions were calculated.

For example, the EU sustainability criteria are extended to cover biomass for heating and cooling and power generation in the revised Directive [EU] 2018/2001. EU countries were required to transpose the new rules by 30 June 2021, and the voluntary schemes have to adjust the certification approaches to meet the new requirements.

For a scheme to be recognized by the European Commission, it must fulfil criteria such as:

- Feedstock producers comply with the sustainability criteria of the revised Renewable Energy Directive and its implementing legislation.
- Information on the sustainability characteristics can be traced to the origin of the feedstock.
- All information is well documented.
- Companies are audited before they start to participate in the scheme and retroactive audits take place regularly.
- The auditors have both the generic and specific auditing skills needed with regards to the scheme's criteria.
- The decision recognizing a voluntary scheme has usually a legal period of validity of 5 years.

If a mixed raw material containing less than 100% biogenic materials is used, the biogenic content shall be calculated according to the share of the biobased materials and reported accordingly. The other share of materials is linked to fossil Carbon.

If a PEF compliant calculation is requested, the PEF figures shall be used.

Table 5.11 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.

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 5.11):

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 pre-cursors, this category is of very low relevance and can be neglected in the evaluation and should be reported as "not applicable".

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], expected to be released end of 2022.

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].

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.

Table 5.12 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

Since there are developments towards new ISO standards, aspects might be addressed differently. On ISO Level there is a new standard, ISO 14068 "Climate neutrality" under development. A Net-Zero approach of ISO started as well with the IWAR 42 Net Zero Guiding principles. These activities might initiate new calculation aspects and implementation of PCF in specific calculations. This guideline will be updated accordingly, when these standards will be published, and new requirements need to be addressed.

5.2.10.4 Carbon Capture followed by Storage, 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 to the capturing of CO_2 at the emissions source only. Direct air capture technologies are out of the scope of this sub-chapter. For other technologies to capture other Carbon sources (e.g. CH_4), further definitions are needed.

CCS (Carbon Capture and Storage, or more accurate: CO_2 capture and storage) refers to the separation of CO_2, and 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 (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, is not covered by the terminology.

Carbon Capture and Storage

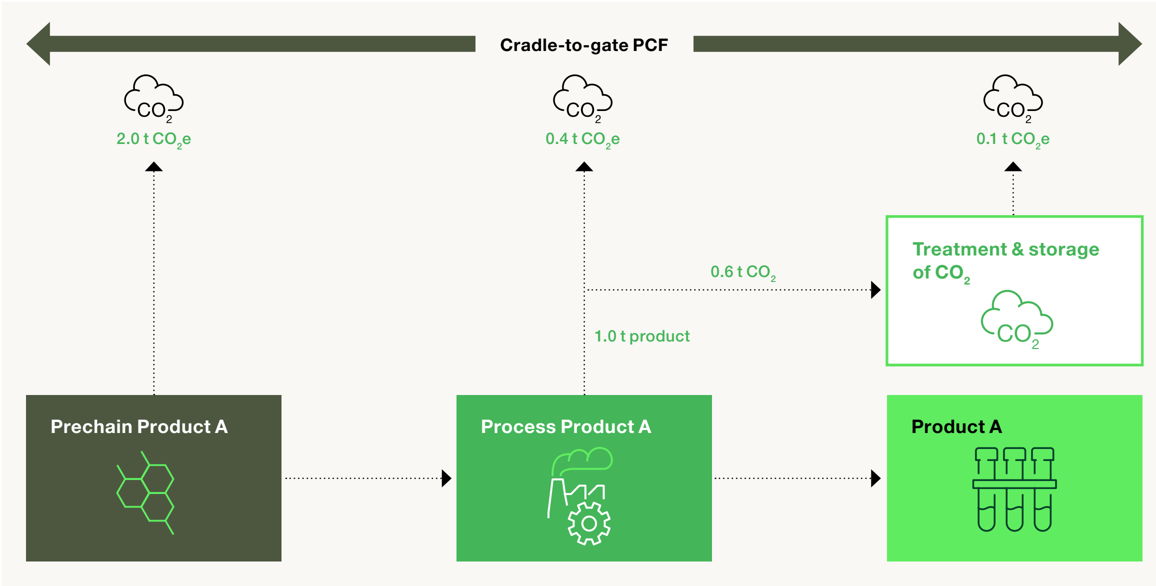
CCS may be included in the PCF calculation if a permanent and complete storage in storage facilities is guaranteed. Permanent storage technologies are characterized by a very low risk of a physical reversal of the storage process. The World Economic Forum offers a comprehensive overview of storing technologies. 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)].

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

Table 5.13 Examples for CCS

Example case (See figure 5.20)	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 5.20)	Absolute values of released emissions and stored emissions can be reported individually

Figure 5.20 Carbon Capture and Storage example (CCS) 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

Without Carbon Capture and Storage, 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

Standards for Product LCAs are currently not harmonized and do not fully address the steering effect of PCFs for important technologies with the potential to de-fossilize the chemical industry, such as carbon capture and utilization and chemical recycling. Thus, the following methodologies are a proposal by the chemical industry to steer for those technologies, but are not harmonized yet with all standards, including the GHG Protocol standard.

Captured CO_2 is a product of human transformation, consequently, CO_2 is a technical flow and a chemical feedstock for CO_2 utilization. When CO_2 is captured and used, ISO- and TfS allocation hierarchy shall be used, meaning that if the multi-output situation cannot be avoided by subdivision, a system expansion or allocation following the approach described in published and accepted product category rules (PCR) or Industry Association projects, where available, for corresponding product systems, shall be applied (see chapter 5.2.9). Both approaches would not be favorable for such a new technology, as shown and explained in the following chapter. Thus, TfS decided to set up an alternative approach to be further discussed and considered.

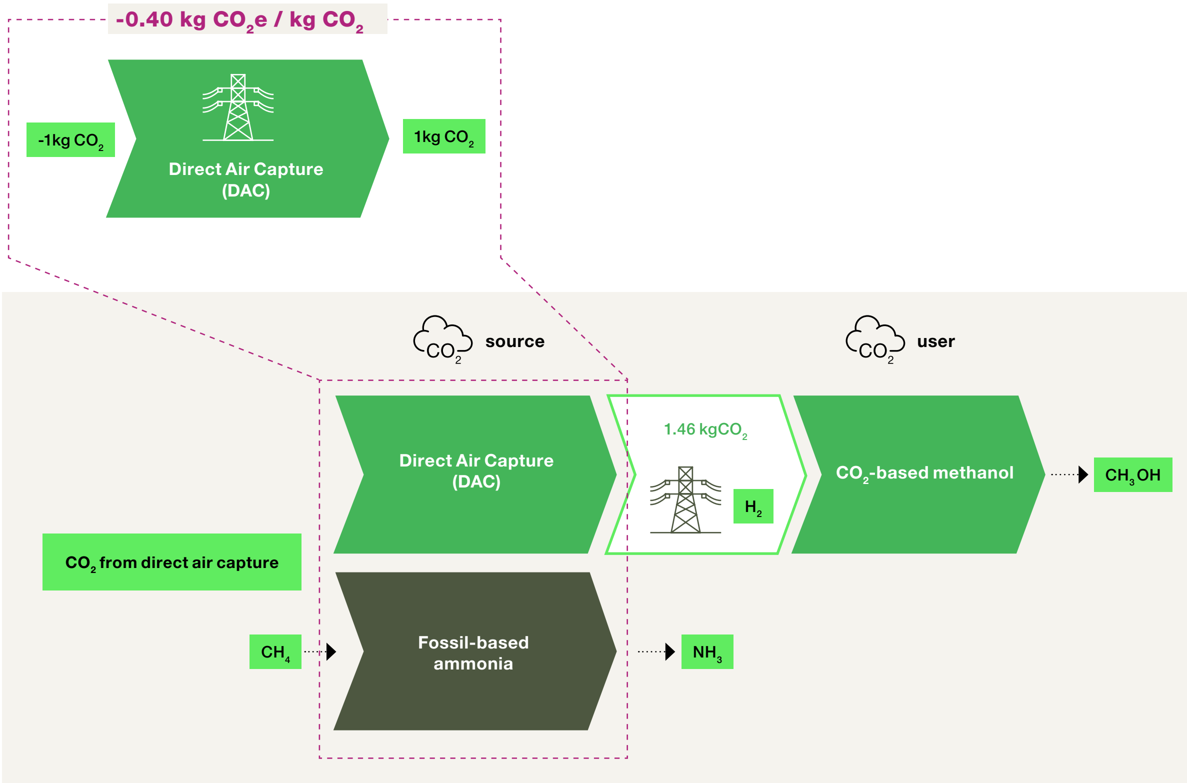
Sources of CO_2 can be either direct air capture (DAC) or point sources (industrial processes like ammonia production). For both sources, the technological transition by capturing and using CO_2 for chemical products is driven by CO_2 users; for point sources, it is also driven by the CO_2 source. The decision-making of CO_2 sources and CO_2 users can only be steered through an assessment methodology that reflects the relationship between main product and the CO_2.

Based on exemplary data as provided in table 5.14, the impacts of different assessment methodologies were calculated for an ammonia plant (as point source) and a methanol production (user of CO_2) as well as a reference CO_2 source from Direct Air Capture (DAC).

Figure 5.21 reflects the results of this cradle-to-gate calculation for CO_2-based methanol with two different sources of CO_2: Direct Air Capture (DAC) and an industrial point source, an ammonia plant. In the exemplary calculation for DAC (see Figure 5.21 and Table 5.14), 1 kg of CO_2 is captured via the DAC. The total PCF related to the CO_2 capturing and the capture process for DAC accounts in this example for 0.60 kg CO_2e/kg CO_2. Including the removal of the 1kg CO_2, the total PCF for captured CO_2 is -0.40 kg CO_2e per kg CO_2. The calculation considers per kg of captured CO_2: 2.52 MJ electricity, 11.9 MJ heat provided via heat pump, which relates to an electricity demand of 4.74 MJ (assumed COP of heat pump of 2.51), and 0.02 kg CO_2e to account for adsorbent losses. In the above example a CO_2e emission factor for electricity of 0.08 kg CO_2e/MJ was used.

In scenario **1) "No multi-output system"**, the methanol process uses 1.46 kg CO_2 from the DAC to produce 1kg CH_3OH. As shown in Figure 5.21, accounting for all emissions from methanol and the raw material H_2 production, the total PCF of the CO_2-based Methanol from DAC accounts 2.57 kg CO_2e per kg CH_3OH. Where DAC is used and thus, no capturing takes place at the ammonia plant, the production of ammonia leads to a PCF of 1.98 kg CO_2e per kg NH_3 (Table 5.14).

Figure 5.21 DAC scenario – The CO_2 is captured in DAC and processed to Methanol. No CO_2 capturing at the ammonia plant (Table 5.15 column 1)



1kg NH_3 + 1 kg CH_3OH = 4.55 kg CO_2e

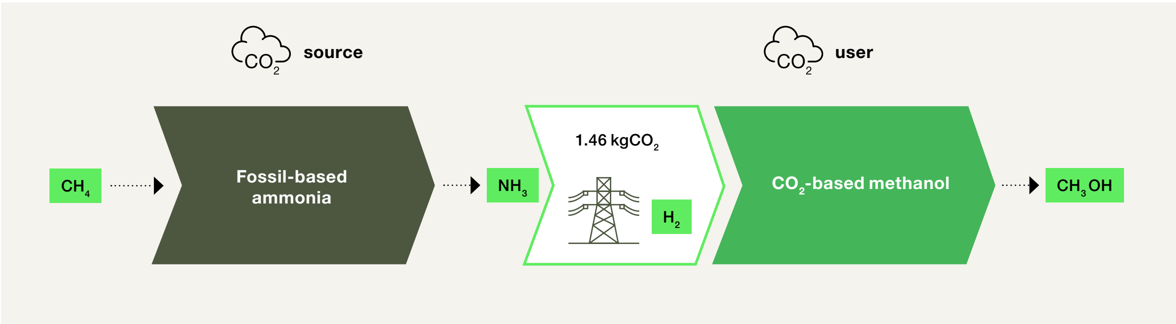
Table 5.14 PCF results using the "No-multi output" approach

Unit: kg CO_2 eq	PCF ammonia as CO_2 source (1kg NH_3)	PCF Methanol as CO_2 user (1kg CH_3OH)	System expansion (1kg NH_3 + 1kg CH_3OH)
CO_2 from DAC	1.98 (no capture)	2.57	4.55

In the case where CO_2 is captured in a point source, the assessment approach influences the PCFs of the ammonia and the methanol. In the following example calculation, the two assessment approaches “system expansion with subsequent substitution of an ammonia plant” and “economic allocation” have been applied to show the impact of different approaches on the PCFs of the two products and thus, the steering effect.

In the scenario **2) “System expansion: avoided ammonia production w/o capture”**, a credit for avoided operation of an ammonia plant without capture is used to determine the PCF of captured CO_2 from an ammonia plant. By this approach, the 1.46 kg CO_2 (needed for production of 1 kg methanol) would leave the Ammonia plant with a PCF of -0.97 kg CO_2 per kg CO_2 captured (-Avoided CO_2 + Emissions from capture = -1 kg CO_2 eq per kg + 0.03 kg CO_2 per kg CO_2). The PCF incentivizes the usage of CO_2 (PCF of CCU-Methanol accounts 1.73 kg CO_2e/kg taking into consideration the negative PCF for CO_2); but does not incentivize the producer of the CO_2, the fossil process of ammonia production. The ammonia production with capture would result in a PCF of 1.98 kg CO_2e/kg NH_3 like in the first scenario of no capture.

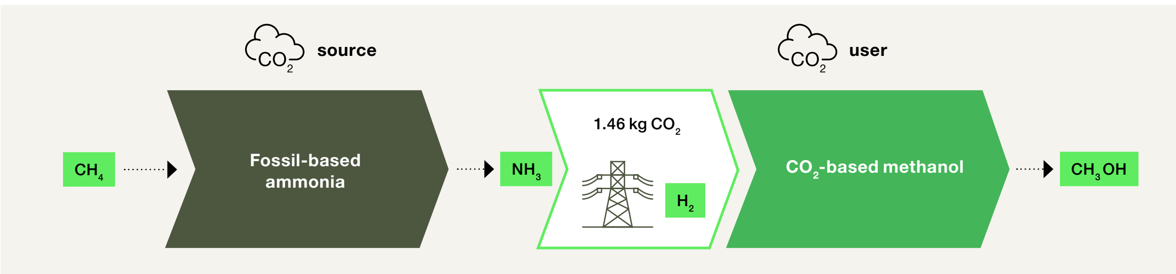
Figure 5.22 CCU from point sources – effects of two different allocation schemes on PCF of Ammonia and PCF of Methanol (Table 5.15 column 2 and 3)



1kg NH_3 + 1 kg CH_3OH = 3.71 kg CO_2e

To avoid this fossil-lock in and to share incentives between both processes (CO_2 source and CO_2 user), TfS is in favor of applying system expansion with substitution of direct air capture (Table 5.15 column 4). As shown in the example below, the ammonia producer can lower the PCF of NH_3 to 1.14 kg CO_2e/kg NH_3. The PCF of Methanol would account to 2.57 kg CO_2e/kg CH_3OH, which is comparable to the DAC scenario and in the average range between system expansion with substitution of an ammonia plant (1.73 kg CO_2e/kg CH_3OH) and economic allocation (3.25 kg CO_2e/ kg CH_3OH). The overall emission of the system is conserved 3.71 kg CO_2e/ (kg CH_3OH + kg NH_3) as for the other approaches. There is a split of incentives between the two products. The approach and rationale of system expansion with substitution of direct air capture is described in the next chapter.

Figure 5.23 CCU from point sources – proposed allocation methodology: System expansion with avoided direct air capture (Table 5.14 column 2 and 3)



1kg NH_3 + 1 kg CH_3OH = 3.71 kg CO_2e

CO_2 capture from point sources is due to their high CO_2 concentrations in general less emission-intensive than direct air capture. The assessment approach for this specific topic should steer CO_2 demand towards CO_2 supply with minimal emissions (from point sources). Thus, CO_2 usage from point sources should benefit from avoiding direct air capture by applying system expansion with upstream substitution of the alternative CO_2 source DAC. Accordingly, the separation of CO_2 from CO_2 point sources and subsequent use in chemicals production should benefit as well because otherwise the CO_2 will be emitted or transferred to storage. The CO_2 point source (e.g. ammonia plant) and the CO_2 user would apply the following calculation logic:

The CO_2 user (here: Methanol plant) applies the PCF of CO_2 of using the best-in-class direct air capture process operated in the region of the point source (in this example: PCF CO_2 = -0.40 kg CO_2 e/kg CO_2 for DAC source). In Table 5.14 column 4, this credit is recalculated with the amount of CO_2 used (1.46 kg CO_2) and thus accounts for -0.58 kg CO_2 e for the methanol production The CO_2 source (here: Ammonia plant) gets the credit of being a more efficient CO_2 capture than the direct air capture process. The PCF for the Ammonia would be reduced by the credit of CO_2 derived from the point source (compared to DAC)., i.e., here:

PCF Ammonia with capture/avoided DAC = Sum emissions Ammonia plant – (PCF avoided DAC * CO_2 -Output Ammonia plant).

In the example this equals

Total per 1 kg NH_3 + 1.46 kg CO_2:
Emissions from Ammonia: 1.58 kg CO_2 - 1.46 kg CO_2 = 0.12 kg CO_2
PCF Ammonia = (0.36 + 0.08 + 0.12) – (-0.58 kg CO_2e) = 1.14 kg CO_2e per kg NH_3

Total per 1 kg CH_3OH:
PCF Methanol = (2.94 + 0.09 + 0.12) + (-0.58 kg CO_2e) = 2.57 kg CO_2e per kg CH_3OH

Table 5.15 Summary overview of assumptions for calculation

		1) No multi-output system	2) System expansion: avoided ammonia production w/o capture	3) Allocation based on economic value	4) Point source Ammonia plant (avoided DAC)
		in kg CO_2e			
Direct Air capture	CO_2 captured (kg CO_2)	1.00	-	-	-
	Contribution electricity direct	0.20	-	-	-
	Contribution electricity for heat	0.38	-	-	-
	Contribution for amine losses	0.02			
	Per kg CO_2	**-0.40[1]**	**-**	**-**	**-**
Ammonia production	CO_2 captured (in kg CO_2)	0	1.46	1.46	1.46
	PCF of captured CO_2 (per kg CO_2)		-0.97	0.07	-0.40
	Contribution captured CO_2 (per 1.46 kg CO_2)	-	-	-	-0.58
	Contribution raw material production	0.36	0.36	0.29[2]	0.36
	Contribution electricity consumption	0.04	0.04	0.07[2]	0.08
	Contribution direct emissions	1.58	1.58	0.10[2]	0.12
	Outputs	1 kg NH_3	1kg NH_3 + 1.46kg CO_2		
	Per outputs	**1.98**	**1.98**	**0.46[2]**	**1.14**
CO_2-based Methanol production	Input CO_2	1.46	1.46	1.46	1.46
	PCF of captured CO_2 (kg CO_2eq / (kg CO_2))	-0.40	-0.97	0.07[2]	-0.40
	Contribution raw material production - CO_2	-0.58	-1.42	0.1[2]	-0.58
	Contribution raw material production - H_2	2.94	2.94	2.94	2.94
	Contribution direct emissions	0.09	0.09	0.09	0.09
	Contribution energy consumption	0.12	0.12	0.12	0.12
	Outputs	1 kg CH_3OH	1 kg CH_3OH		
	Per output	**2.57**	**1.73**	**3.25**	**2.57**
	Per (1 kg NH_3 + 1 kg CH_3OH)	**4.55**	**3.71**	**3.71**	**3.71**

(1) PCF CO_2 lowered by capture energy, which needs to be considered
(2) Economically allocated emissions-based price Ammonia (380 EUR/ton) and price CO_2 (60 EUR/t). Source: https://pubs.rsc.org/en/content/articlepdf/2020/ee/d0ee01530j

The PCF for CCU processes calculated in accordance with this TfS guideline shall use system expansion with avoided DAC. For the calculation of the PCF of captured CO_2, the following energy demand shall be considered: 2.52 MJ electricity per kg CO_2 captured and 4.74 MJ of electricity that are used for the provision of low temperature heat (>100°C) via a heat pump [Deutz 2021]. Additionally, 0.02 kg CO_2e per kg of captured CO_2 shall be considered to account for adsorbent losses during air capture. Note that in the examples above a CO_2e emission factor for electricity of 80 g CO_2 e per MJ of electricity was used. This factor shall be adjusted to reflect the electricity consumption mix of the country where the CO_2 producer is located. The following formula shall be used:
PCF of 1kg captured CO_2 = 0.02 kg CO_2e +(2.52 MJ +4.74 MJ) *spec. emission factor electricity – 1kg CO_2.

It must be noted that in LCA databases, life cycle inventories of multi output systems are often modelled differently following deviating allocation principles (e.g., physical allocation versus economic allocation) or system expansion followed by substitution. Therefore, when selecting secondary data sets, care must be taken to ensure that they comply with the allocation principles as defined in this guideline. If these are not available, they must be developed with the database providers, if possible, to achieve harmonization. Otherwise, the result of the PCF calculation also depends on whether a supplier-specific data set from a chemical company that adheres to the principles of this guideline, or a secondary data set was used. The modeling approach for systems with CCU (system extension with avoided direct air capture) suggested in the guideline is not yet reflected in the existing LCA databases with the consequence of creation of different results. A meaningful reporting that shows the calculation approach shall be linked to the figures also for comparison of different PCF of CCU products.

5.2.10.5 Calculation of mass-balanced products

Mass balance is a chain of custody used in multiple industries in which it is not practical to maintain physical segregation of alternative and conventional materials 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. Alternative materials can be e.g., bio-based feedstocks but also other feedstocks such as chemically recycled feedstocks, waste feedstocks or CO_2-based materials. Mass balance is especially important to many companies in the chemical industry who are transitioning to use of waste plastic and bio-based materials as feedstocks to reduce the usage of virgin fossil-based materials and to help solve the global plastic waste dilemma with molecular recycling. Mass balance does require a physical link between input and outputs materials and is therefore different from more indirect chain of custody approaches such as Book and Claim.

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 to create value from the use of alternative inputs. Large integrated assets cannot be transitioned immediately, and mass balance provides a critical bridge.

The mathematical approach to calculating PCF for processes in which mass balance attribution occurs is beyond the scope of this guideline because it is different for different types of chemical processes. An industry guidance, product category rule, or international standard is needed for implementation of mass balance in LCA. It is not possible to standardize an approach in this TfS guideline for this complex and emerging topic. Further standards development on chain of custody considerations in LCA is needed.

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.

   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.

2. The LCA of 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 bio- or bio-circular attributed raw materials the biogenic uptake can be considered, but double counting shall be avoided. (e.g. biogenic uptake has to 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-balance products the term biogenic carbon content should be enlarged to biogenic carbon content/ attributed biogenic carbon (acc. to the mass-balance approach).

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 using pyrolysis followed by steam cracking. The concept conforms to the requirements ISO 14044 [ISO 14044: 2006] and may be applied to mass balance applications using bio-based feedstocks (biomass balance) or recycled feedstocks (circular mass 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) are determined based on relative conversion rates of the different feedstocks and chemical values of the resulting outputs.

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 should be determined (and shared) [Pathfinder Framework (PACT powered by WBCSD)]. This can be done by calculating the proportion (%) of the total GHG impact (CO_2 eq) that is derived by using primary data in the cradle-to-gate system boundary (see Formula 2). See glossary for definitions of primary and secondary data.

Formula 3: Calculation approach of the PDS

$$\frac{\text{Part of PCF based on primary data } (CO_2e)}{\text{PCF } (CO_2e)} = PDS_{PCF}(\%)$$

Ideally, the share of primary data for relevant input flows obtained from upstream suppliers (tier n-1) are available. If so, the PDS of the PCF should be calculated using a PCF attributed average approach of the material and energy inputs. If not all members of the supply chain are encouraged to participate in this effort as the share of primary data can only be accurately determined if the respective information for most inputs is provided by the respective suppliers.

To do so, the individual PDS received from supplier (PDS external components) as well from other components (PDS other components), e.g., energy inputs or direct emissions from production, should be multiplied with their respective relative contribution (in %) to the PCF. All weighted PDS (weighted PDS components) should then be added up to obtain an overarching PDS (PDS output). To help increase transparency on primary data use, information on PDS should be shared downstream (tier n+1) together with the PCF. 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 and ensuring more accurate PCFs if the quality of the data is in addition very good (Figure 5.24). The general approach is shown in Figure 5.25.

Figure 5.24 Calculation of Primary data shares of two components

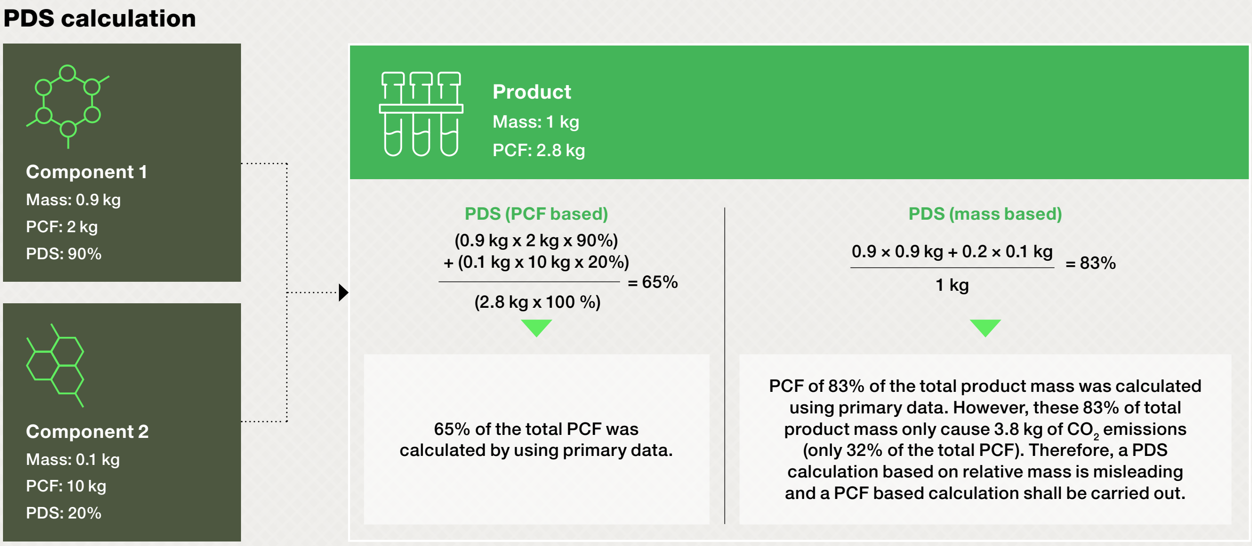
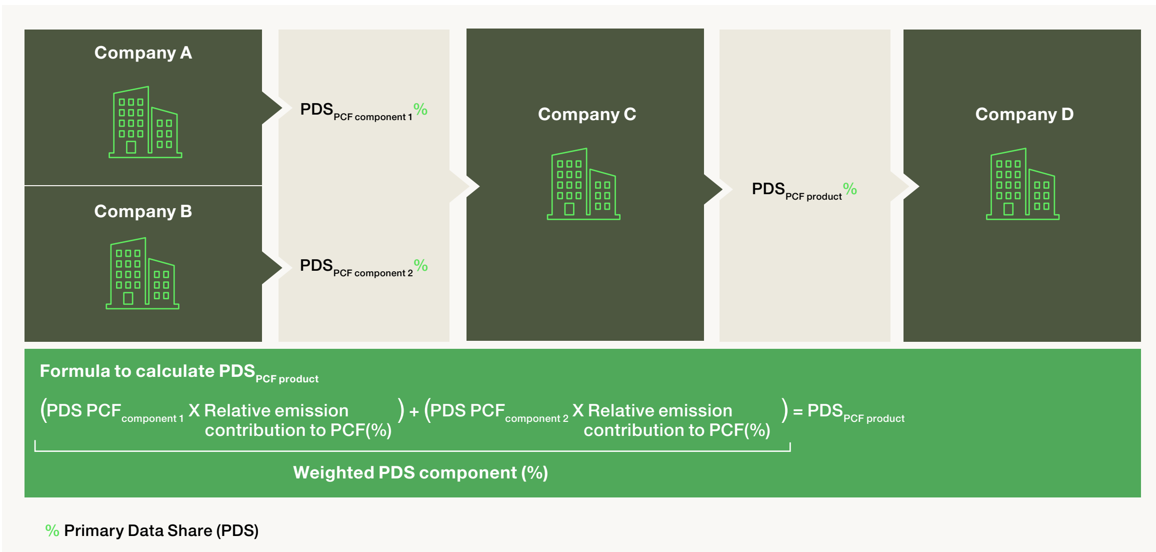
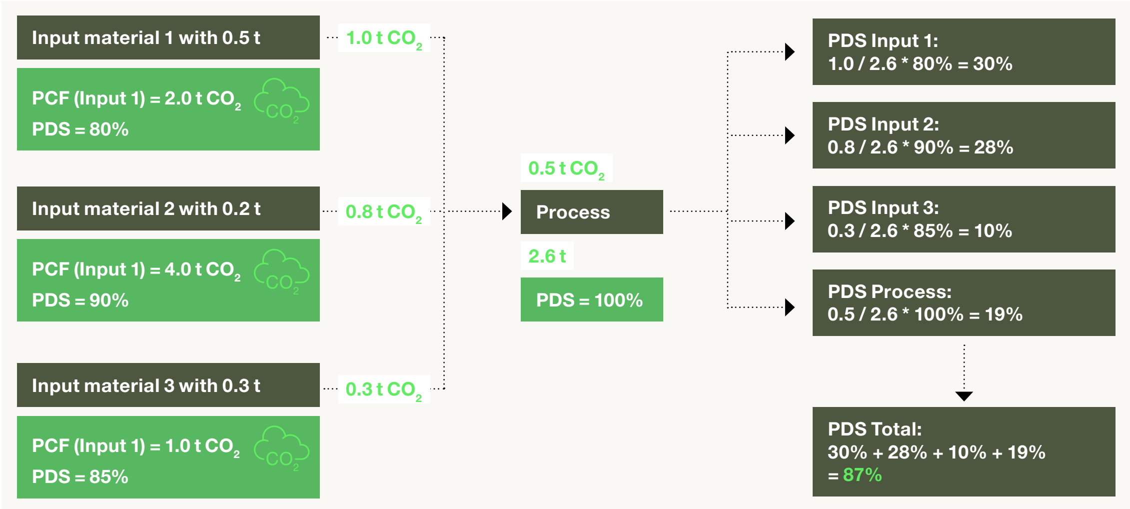


Figure 5.25 Calculation of Primary data share for a PCF [Pathfinder Framework (PACT powered by WBCSD)]



A detailed example is shown in Figure 5.26 with application of detailed steps in the generation of 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 is derived from primary sources. If one of these two information is derived from secondary data, the whole PDS for this unit process is rated as secondary data.

Figure 5.26 Calculation of Primary data share for a PCF, example



In general, a primary dataset can only be rated as primary, if the activity data (data source) and the emission factor (EF source) is a primary information. If only one of the two factors of the PDS calculation is secondary, the whole rating for this contribution is rated as secondary and will be implemented in the PDS calculation accordingly. An example is given in Table 5.15.

Table 5.16 PDS calculation example for primary and secondary data sources

Material	Data input (kWh)	Data source	EF (kg CO_2e)	EF source	kg CO_2e	% PCF	Total PDS
A	10,435	Primary	0.19	Primary	1,983	42%	42%
B	10,000	Secondary	0.18	Secondary	1,800	38%	0%
C	5,000	Primary	0.18	Secondary	900	19%	0%
					4,683		**42%**

5.2.11.2 Data quality rating (DQR)

During the data collection process, companies shall assess the data quality of activity data, emission factors, and/ or direct emissions data by using the data quality indicators.

If higher-quality data exists in-house than available in secondary databases (for example, in-house emission factors for fuel) and is used for calculations, the adequacy of such in-house data shall be reviewed and reported in a DQR following the criteria outlined in 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 becomes mandatory only from 2025 on to give companies enough time to prepare for this. Until then it is recommended to do it on a voluntary basis.

The standard defines five data quality indicators to use in assessing data quality. They are shown below and summarized in Table 5.16.

- **Technological representativeness:** the degree to which the data reflect the actual technology(ies) used in the process.
- **Geographical representativeness:** the degree to which the data reflects actual geographic location of the processes within the inventory boundary (e.g., country or site).
- **Temporal representativeness:** the degree to which the data reflect the actual time (e.g., year) or age of the process.
- **Completeness:** the degree to which the data are statistically representative of the process sites.
- **Reliability:** the degree to which the sources, data collection methods, and verification procedures used to obtain the data are dependable.

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.

The Pathfinder Framework requires only those inputs representing more than 5% of the total PCF to undergo the DQR assessment which reduces the workload for the generation of DQR factors. TfS recommends this approach as well (Table 5.17).

Table 5.17 Data quality indicators of GHG Protocol

Indicator	Description	Relation to data quality
Technological representativeness	The degree to which the data reflects the actual technology(ies) used.	Companies should select data that are technologically specific.
Temporal representativeness	The degree to which the data reflects the actual time (e.g., year) or age of the activity.	Companies should select data that are temporally specific.
Geographical representativeness	The degree to which the data reflects the actual geographic location of the activity (e.g., country or site).	Companies should select data that are geographically specific.
Completeness	The degree to which the data are statistically representative of the relevant activity. Completeness includes the percentage of locations for which data is available and used out of the total number that relate to a specific activity. Completeness also addresses seasonal and other normal fluctuations in data.	Companies should select data that are complete.
Reliability	The degree to which the sources, data collection methods and verification procedures [1,2] used to obtain the data are dependable.	Companies should select data that are reliable.

(1) Adapted from B.P. Weidema, and M.S. Wesnaes, "Data quality management for life cycle inventories - an example of using data quality indicators," Journal of Cleaner Production. 4 no. 3-4 (1996): 167-174.
(2) Verified data: Verification may take place in several ways, e.g., by on-site checking, by recalculation, through mass balance, or by crosschecks with other sources.

Table 5.18 Data quality assessment used in TfS and [Pathfinder Framework (PACT powered by WBCSD)]

DQI	1 - Good	2 - Fair	3 - Poor
Technology	Same technology	Similar technology (based on secondary data)	Different or unknown technology
Time	Data from reporting year	Data less than 5 years old	Data more than 5 years
Geography	Same country or country subdivision	Same region or subregion	Global or unknown
Completeness	All relevant sites for specified period	<50% of sites for specified period or >50% of sites for shorter period	Less than 50% of sites for shorter time period or unknown
Reliability	Measured activity data	Activity data partly based on assumptions	Non-qualified estimate

The quality assessment of data based on the Table 5.14 can be used to derive more quantitative information in form of a Data Quality Rating (DQR) to give users of the data a better impression of the overall quality of data and the resulting PCF.

The data quality of each PCF shall be calculated and reported. The DQR calculation shall be based on five data quality criteria (each criterion considered of equal importance) where TeR is the Technological-Representativeness, TiR is the Time/Temporal Representativeness, GeR is the Geographical-Representativeness, C is completeness and R is reliability.

The quality levels are expressed in three categories from, 1 Good, 2 Fair, 3 Poor. The representativeness (technological, geographical, and time-related) characterizes the degree to which the processes and products selected depict the system analyzed, while the completeness and reliability addresses the quality of the generated PCF result.

The contributions of the input materials to the PCF of the process are linked with the DQR of the input material. As lower the DQR score and as higher the share of the total PCF for an input material is, as more positive is the impact of an input material to the overall DQR_{total} score.

For example:	Product 1	Product 2
Technological representativeness (TeR):	2	3
Temporal representativeness (TiR):	1	3
Geographical representativeness (GeR):	2	2
Completeness (C):	3	3
Reliability (R):	2	3
Total	**10**	**14**
DQR Process (Total / 5)	**2**	**3**

In Formula 4, the aggregation of all single results of all input materials from upstream is shown. The second line shows the general calculation of a single DQR of a process, based on the five criteria described above. In line 4 it is shown, how to add process related DQR and the upstream DQR according to Figure 5.27.

Formula 4: General calculation of data quality ratings

$DQR_{upstream}$ = (DQR Inputmaterial 1* PCF_{total} share 1+ DQR Inputmaterial 2* PCF_{total} share 2 + DQR Inputmaterial 3* PCF_{total} share 3+ DQR Inputmaterial n* PCF_{total} share n)

$DQR_{process}$ = (TeR + TiR + GeR + C + R) / 5

$DQR_{process}$ contribution = $DQR_{process}$ *PCF_{total} share process

DQRtotal = ($DQR_{upstream}$ + $DQR_{process}$ contribution)

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

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 2025. 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. Note that the DQR of the process is not always equal to 1 depending on which data are available. A process where primary data can be generated, can always have a low Technological or Temporal representativeness ending in lower scores than 1. Company owned processes must be assessed in the same manner as upstream processes.

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 re-collect data [GHG Protocol Product Standard].

The following steps are useful when improving data quality:

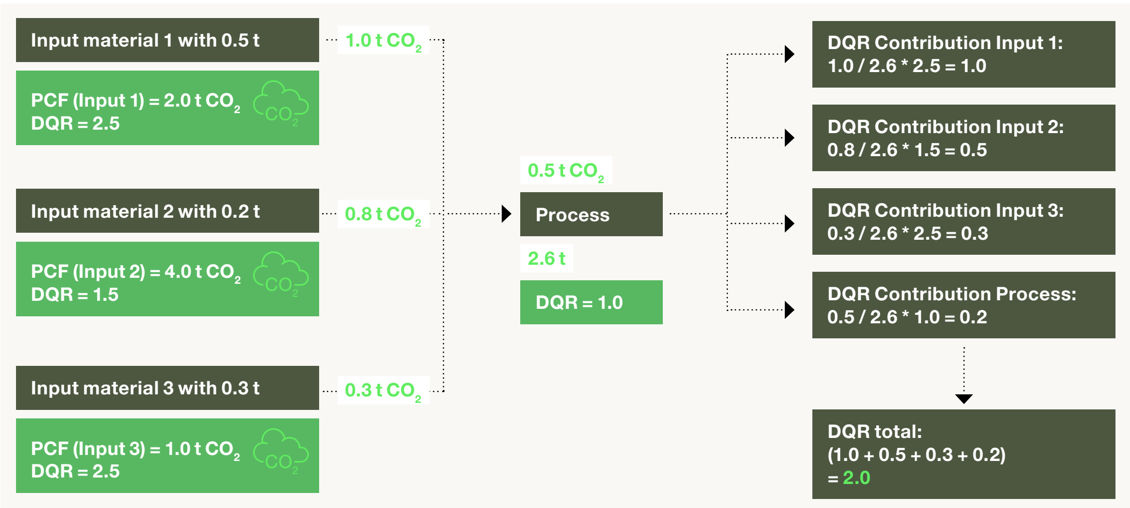
1. Identify sources of low-quality data in the product inventory using the data quality assessment results. Sources with low quality data that have been identified as significant to the PCF results should be given priority.

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.

Figure 5.27 DQR example for a process including upstream DQR (Source TfS)



5.3 Verification and reporting

Table 5.19 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 sold 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

5.3.1 Verification of PCF calculations / Quality assurance

A **verification** is defined as the confirmation, through the provision of objective evidence, that specified requirements have been fulfilled [ISO 9000: 2005]. To achieve the verification, the calculations shall be cross-checked against the requirements of this guideline and the results shall be reported.

Verification of PCF data prior to sharing is strongly encouraged to ensure high quality and trustworthy data [Pathfinder Framework (PACT powered by WBCSD)]. A significant update has been made to the verification and assurance chapter within the Pathfinder Framework.

No verification is not allowed under TfS. Possible types of verification can be an internal LCA expert, a third party verification - product review or a independent party verification - systematic approach review. The type of verification must be reported together with the PCF (see 5.3.2).

If internal verification is done, the claim of the PCF figure shall always include that the PCF was calculated in alignment with the TfS Guideline, while a third-party verification allows a stronger claim (e.g. verified against TfS)

Any type of verification should include a 4-eye-principal check by an internal LCA expert or external auditor regarding the following aspects:

- The goal and scope and its related aspects (see 5.1).
- The calculation rules (see 5.2).
- The system boundaries (see 5.1.2 and cut-off criteria (see 5.2.3).
- The data quality (see 5.2.5).

A third-party verification can be helpful, to fulfill these requirements. This can either be done on a product level or in a systematic approach verification where a company methodology to calculate consistent PCF is verified.

The **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, if the PCF results and the approach to achieve them fulfills requirements of high quality beyond data quality (adopted from [ISO 9000: 2005]).

The following short checklist can help the LCA practitioner to validate the PCF. Besides the LCA expert, people that 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 as well as emissions into air and water).
- 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 if the carbon balance is closed, all inputs are considered and balanced with outputs to products, emissions (air, water, soil), wastes. Check if process related direct emissions are plausible (carbon, nitrogen process input output balances).
- Check data aggregation, data polishing and underlying modeling to calculate product inventory of your own data sets.
- Check if correct calculation formulas where applied.
- Check utility consumption (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.
- CO_2e benchmark against own calculations, same product from other sites/plants companies, existing LCA data, LCIs from 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 is the appropriate.
  - Check if the application of proxies is appropriate.
  - If supplier data is available replace dataset.

- Check if a data quality score was generated and if it is meaningful.
- Check why there are significant deviations to LCA benchmark data.
- Sensitivity analysis and quality checks of results: Sensitivity analyses with different modeling choices (e.g., another dataset for a raw material, another allocation method for the foreground product system) should be performed to test the robustness of the result.
- A variation of 10% of the PCF result by including or excluding life cycle stages is a variation that is mainly 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 for their 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 or attached to complement and provide more details to the information [BASF SE (2021)].

Results reported in the PCF study report may be used in footprint communications [ISO 14026: 2017].

5.3.2 Information to be reported with PCF

This section specifies the information requirements to be provided by suppliers alongside PCF values. Additional information besides 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. 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 given. Comparisons of PCF are only possible under certain criteria if all relevant information is reported.

The fields marked as “mandatory” in the table 5.19 (“yes”) shall be provided by suppliers when disclosing PCF values. Some fields will become mandatory from 2025 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 provide further support. ISO 14067 [ISO 14067: 2018] describes requirements for reporting which are reflected in the attributes list. To be fully compliant for a PCF study, all reporting requirements shall be addressed. In the B2B exchange, if no further information is requested, the following GHG values shall be the basis for a PCF study report:

- Declared unit.
- Total GHG emissions and removals. Optional their link to the main life cycle stages in which they occur, including the absolute and the relative contribution of each life cycle stage.
- Net fossil GHG emissions and removals.
- Biogenic GHG emissions and removals.
- GHG emissions and removals occurring because of land use and direct land use change.
- Biogenic carbon content of products.
- Functional or declared unit and reference flow.
- The selected cut-off criteria and cut-offs.
- The selected allocation procedures.
- Description of data and data quality.
- Treatment- and use of electricity.
- Description of the stages of the life cycle.
- Time period for which the PCF is representative.
- A graphical presentation of results of the PCF.
- Where an aviation multiplier is used, the effect of this multiplier shall not be included in the PCF and shall be reported separately together with the source.

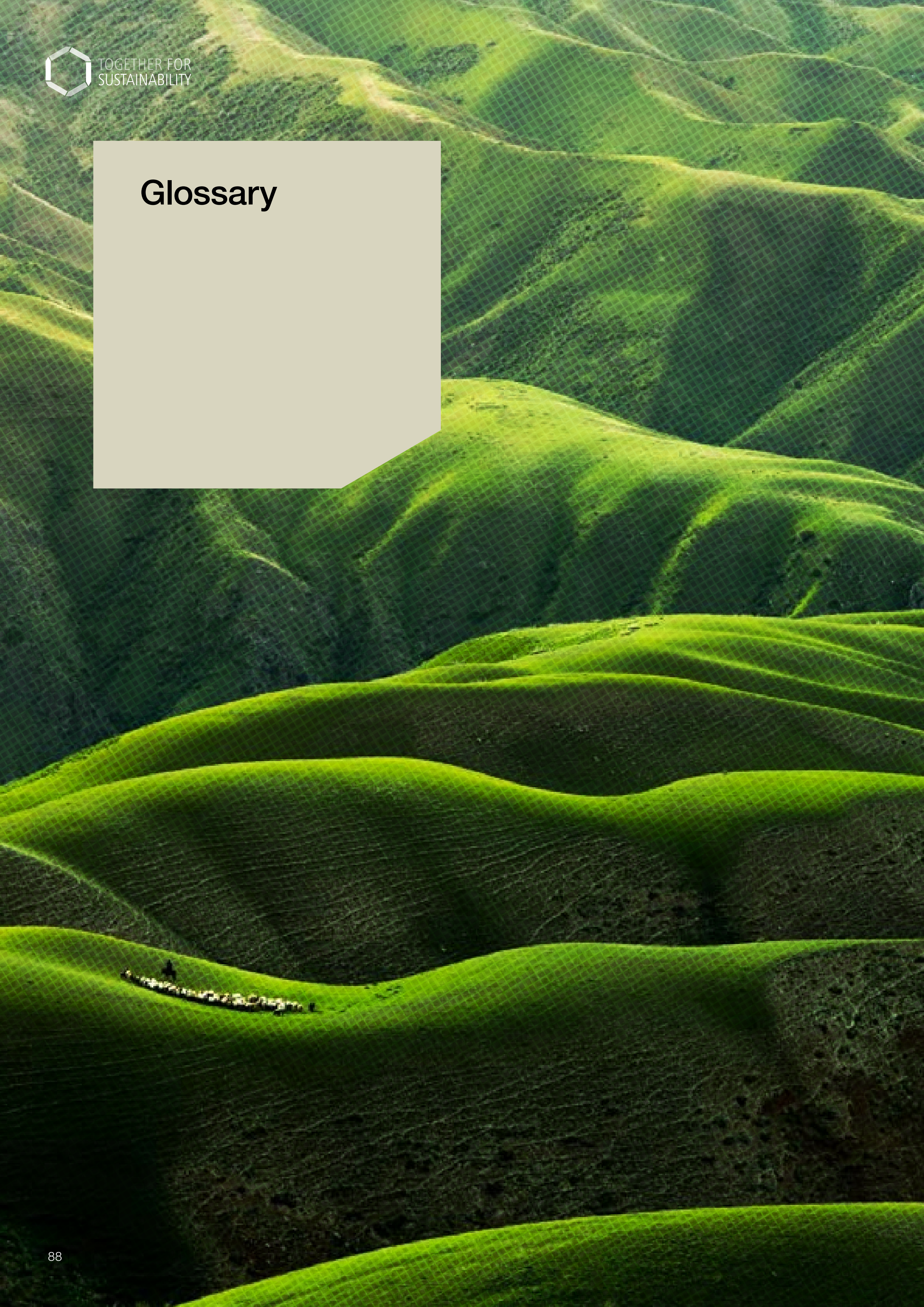
Table 5.20

Category	Attribute	Further explanation (Semantics and ILCD)	Example	Mandatory
Company and product	Company name	(Legal) Name of Data owner	My corp	yes
	Company ID	Abstract ID	E.g. # 311	yes
	Product trade name	Product name	Green Ethanol	yes
	CAS	CAS Number	58-08-2	yes, if available
	Declared unit: kg	Unit of analysis of the product (always kg)	1 kg	yes
	Product description including reference to the solution for which PCF is reflected	(Technical) description of product or waste	Ethanol, 95% solution	yes
PCF	Unique ID	ID of exchanged PCF, e.g. UUID	58-08-2-0017	no
	PCF (excl. Biogenic emissions and removals)	Cradle-to-gate PCF in kg CO_2e/kg product Sum of separate emission values 1 + 2 + 3	2.6 kg CO_2e/kg Ethanol	yes
	PCF (incl. biogenic emissions and removals)	Cradle-to-gate PCF in kg CO_2e/kg product Sum of separate emission values 1+2+3+4	0.7 kgCO_2e/kg Ethanol	yes, from 2025 on
	Separated into emission values: 1. Fossil CO_2e-emissions (net result of fossil emissions and removals) 2. Biogenic CO_2e-emissions (only other GHG emissions than CO_2 – excludes biogenic CO_2) 3. Land use and direct land use change CO_2e-emissions 4. Biogenic removals (biogenic CO_2 contained in the product) 5. Aircraft CO_2e-emissions	In kg CO_2e/kg product	1. Fossil CO_2e: 2.0 kg CO_2e/kg Ethanol 2. Biogenic CO_2e*: 0.4 kg CO_2e/kg Ethanol 3. Land use /LUC CO_2e: 0.2 4. Biogenic removal: -1.9 kg CO_2e/kg Ethanol 5. Aircraft CO_2e: 0.0 kg CO_2e/kg	Separated emission values: yes, from 2025 (at least 1, 2-4 only if applicable) Please keep in mind that reporting is mandatory if a compliance with ISO 14067, PEF or the Pathfinder is anticipated
	Total carbon content	Kg C/kg product	0.521 kg/kg Ethanol	yes
	Reference period (year or start/end date if > one yr) and version (if revised within reference period)	Year/period of PCF calculation	2021, v 2.0 Or 01/01/2020 – 31/12/2021	yes
	Geography (as specific as possible)	Location of production / product	Global, Europe, Germany, or Ludwigshafen, 67063, Germany	yes

* If the share of biogenic CO_2 emissions is not known and cannot be determined, the calculated CO_2 emissions shall be considered as fossil CO_2 emission. In this case the CO_2 removal shall only be calculated based on the carbon content in the product.

Category	Attribute	Further explanation (Semantics and ILCD)	Example	Mandatory
	Technological reference *	Technological description	Electrolysis	yes, from 2025 on
	Data quality rating (DQR)	DQR in score from 1 to 3	DQR 1.5	yes, from 2025 on
	Primary data share (PDS)	PDS in %	PDS 95%	yes, from 2025 on Please keep in mind that reporting is mandatory if compliance with Pathfinder is anticipated
	Source of secondary data and version	Refers only to source of secondary data at reporting company	ILCD, Carbon Minds, ecoinvent 3.8, open sources	yes
	Allocation method used *	Type of allocation	Mass allocation	yes
	Verification approach (None, Internal LCA Expert, Third Party Verification - Product Review, Third Party Verification - Systematic Approach Review)		Verification by internal LCA expert	yes
Boundary & standards	PCF calculation Standards or guidelines used (or product or sector specific rules if used)	Standard used for calculating the PCF	PCR, TfS Guideline 2022, ISO 14067: 2018	yes
Additional information – biobased materials	Biogenic carbon content (physical or BMB)	Kg Bio-C/kg product	0.52 kg biogenic C/kg Ethanol	yes, from 2025 on
Additional information – waste incineration	Allocation approach used for waste incineration with energy recovery	Cut-off, reverse cut-off or system expansion		yes
Additional information – chemical recycled material	Recycled carbon content (physical or BMB)	Kg recycled-C/kg product	0.5 kg recycled C /kg Ethanol	no
	Allocation method used for recycled carbon content		Upstream System expansion or cut-off	no
	Type of recycled content		Post-industrial, post-consumer	no
Additional information – Captured and used CO_2 material	CCU-based carbon content	Kg CCU-C/kg product	0.5 kg recycled C/kg Ethanol	no
	Allocation method used for CCU		System expansion and substitution	no
	CO_2-origin	Source from where CO_2 is captured	DAC or Point source ammonia plant	no
Additional information – transportation	CO_2e-emissions from transportation between producer and customer	Kg CO_2e per kg product	0.08 kg CO_2e/kg	no
Additional information – general	Further information on modelling	Assumptions and limitations	Cut-off set on 6%	no

* Of the foreground system, i.e. the last process in the value chain that is calculated.



Glossary

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 in order 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.

(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	

Abbreviation	Term	Definition
kg	kilogramm	
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 Organisation.
	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]
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 4.2
	Production mix	This approach focuses on the domestic production routes and technologies applied in the specific country/region and individually scaled according to the actual production volume of the respective production route. This mix is generally less dynamic.

Abbreviation	Term	Definition
	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]
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
	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:
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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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