business solutions for a sustainable world

Life Cycle Metrics for Chemical Products

A guideline by the chemical sector to assess and report on the environmental footprint of products, based on life cycle assessment

wbcsd chemicals

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We are delighted to present this new publication from the World Business Council for Sustainable Development (WBCSD)'s Chemical Sector Project: "Reaching Full Potential".

This is the Project's third publication after "Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain" (2013) and "Addressing the Avoided Emissions Challenge" (2013).

These guidance documents share a common objective – to provide guidelines and metrics for consistent and credible communication on how the value chains of chemicals impact on and contribute to sustainability.

As a solution provider, the Chemical Industry is an enabler of improved sustainability across value chains, and the companies that are a part of the Reaching Full Potential Project fully embrace this role. To get true market pull for more sustainable products and to realize the WBCSD's Vision 2050 – 9 billion people living well within the limits of the planet – there is a need to provide and communicate information on the sustainability performance of products that customers and stakeholders can trust and compare, to enable them to make informed sustainable choices.

Metrics are vital in order to make informed decisions. They enable companies to understand, improve and evaluate the environmental impact and benefits of their products.

This new guidance focuses on life cycle assessment (LCA) methods to assess the environmental footprint of products. Reporting at a product level, rather than at a chemical company level, provides a useful perspective to decision-makers in the value chain.

The next step will be to develop guidelines to assess the impacts and benefits of chemical products from a social perspective. This work was recently started and should be ready by late 2015.

Just as in our previous work, we encourage our value chain stakeholders to engage with us so as to further improve the guidelines and quality of our methodology. This is vital if we are to make a tangible difference to sustainable development.

Mr. Ton Büchner, CEO, AkzoNobel

"AkzoNobel is committed to work towards a more sustainable world. By collaborating with peers and partners in WBCSD to agree shared and transparent life-cycle metrics and tools we can be sure to compete on customer solutions and performance, rather than methodology."

Büchner

Mr. Feike Sijbesma, CEO, Royal DSM

"In order to move towards a truly sustainable society, we need to speak the same language and work with harmonised life cycle metrics, providing well defined, consistent and trustworthy information to all participants in the value chain, including consumers."

Dr. Klaus Engel, CEO, Evonik Industries

"Sustainability plays an important role for our customers. They expect the products and technologies they receive from us to comply with high environmental and social standards while also being cost-efficient. By developing constantly improved solutions, we are strengthening the trust our customers place in us. For example, we have proved through certified life cycle assessments that the addition of amino acids to animal feed not only provides balanced nutrition but also saves resources and the environment."

Klaus Engel

Mr. Jean-Pierre Clamadieu, CEO, Solvay

"Developing more sustainable products is part of our responsibility as a chemical company and is at the heart of Solvay's strategy. By helping our stakeholders to better understand our product's environmental footprints, these guidelines will stimulate industry's innovation towards a more sustainable chemistry."

Dr. Kurt Bock, Chairman of the Board of Executive Directors, BASF SE

“At BASF, we have anchored sustainability in our corporate strategy. We combine economic success with environmental protection and social responsibility. With chemistry as an enabler we help our customers to meet current and future needs of society. To improve the sustainability of products and processes, we are using tools that examine their entire life cycle. We appreciate a global framework to align environmental footprinting of chemical products. This will ensure the communication of consistent environmental information along the value chain.”

Mr. Godefroy Motte, Senior VP and Chief Sustainability Officer, Eastman Chemical

“Sustainability is about making balanced choices and contributing solutions that are right for business, society, and the world. However, this needs to be done across the value chain to ensure that we design and manufacture these products in a responsible way. Life cycle thinking is a mindset we need to embed in our innovative chemistry and materials product development. Rigorous tools such as product life cycle assessment are vital to generate insights and promote a more holistic understanding of the environmental benefits, burdens, and trade-offs of competing solutions. This is the way to make balanced choices that are critical to both current and future generations.”

Mr. Kasper Rorsted, Chief Executive Officer, Henkel

“We believe that sustainability will be more important than ever before to develop our business successfully. By 2050, global population is expected to climb to 9 billion. This growth will go hand in hand with the changing consumption patterns of a growing, more affluent middle cla ss in emerging markets. At the same time, natural resources such as fossil fuels and water, which are already stretched, will be even more limited.”

Dr. Yoshimitsu Kobayashi, President and Chief Executive Officer, Mitsubishi Chemical Holdings Corporation

“Only through integrating and embedding the management of sustainability into our existing management system with a sense of urgency, can we commit ourselves to long-term balanced growth within the limits of our small planet. No matter how complex or difficult, adoption of Life Cycle Assessment must be promoted among businesses and communities so that it can be applied to each individual economic activity.”

Mr. Mohamed Al-Mady, Vice Chairman & Chief Executive Officer, SABIC

“To improve something, you need to be able to measure it. Life Cycle Assessments of the environmental impact of a product allow us to take sustainability into account and therefore make the best possible business decisions”.

Mady Mohamed

Mr. Cholanat. Yanaranop, President, SCG Chemicals Company Limited

“SCG Chemicals aims to be one of regional market leader, contributing to the sustainable progress of ASEAN, and local communities where we operate.”

cefic

These guidelines have been developed with the support and contribution of the European Chemical Industry Council (cefic)

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1. Executive summary

Why define common metrics for the chemical product footprint?

The chemical industry innovates and produces products that are part of the life cycle of the majority of everyday goods. The position of the chemical industry in the value chain is therefore unique in enabling a reduction in environmental impacts and improving the social performance of countless goods. To assess the contribution of chemical products to impacts (and to impact reductions), chemical companies have invested substantial effort in studying the environmental impacts of various products. **The objective of this guideline is to promote consistent and credible assessment and communication on the environmental life cycle impact of chemical products for value chain partners. This document provides state-of-the art guidance for the chemical industry globally.**

Life cycle assessments (LCAs)[1] are used extensively by the chemical industry for internal support and strategic decision-making, as well as for communication with stakeholders. However, due to the range of currently available methodological choices, the use of existing LCA standards and guidelines does not guarantee comparable results. This document outlines guidance for chemical companies to measure and report the environmental life cycle impacts of chemical products.

Provided that LCAs are used correctly, following international standards and guidelines, they can be a powerful tool that enables environmental impacts to be considered in product strategies. As the most recognised method of assessment, they enable consistent and credible assessment and comparison of the environmental performance of products, identification of improvement opportunities and informed decision-making.

The continual efforts of the chemical industry to assess products require robust, powerful and comparable assessments that are accessible to all stakeholders.

In a second phase of this project, further work will be devoted to social impact assessment.

Value of this guidance

This guidance reflects the best practices used to consistently carry out LCAs and report the environmental footprint for chemical sector products, although it is inherently limited by the current state of development of some methodologies.

1. Pioneering

Building on the best, well-established methodologies and standards, this guidance is the **first global and sector-specific guidance for consistent assessment and reporting of a chemical product's environmental life cycle footprint.**

2. Ensuring comparable and credible environmental impact assessment

This guidance provides a common assessment methodology. If used consistently, it will **increase the comparability of chemical product assessments in terms of environmental performance**. This guidance aims to drive and support consistent and credible product LCA claims across companies and across sectors.

3. Anticipating value chain needs

This guidance reflects the ambition of the chemical sector **to improve and facilitate environmental impact assessments and decision-making for other companies down the value chain.** Such companies can rely **on consistent upstream and downstream information** on the environmental performance of the chemical products they use to develop and eco-design their own sustainable products.

4. Engaging stakeholders

The process to develop this guidance included input from relevant **internal and external chemical sector stakeholders**, ensuring product environmental assessment and communication meets their expectations.

5. Providing practical and educational guidance

This guidance is **designed to be user-oriented**, providing pragmatic guidelines and case studies to be used for specific chemical products. Particular attention has been dedicated to the readability of the document, both in terms of technical vocabulary definitions and illustrative examples.

6. Calling for action

The development of this guidance highlighted **critical gaps** (in terms of uncertainties regarding some impact assessments, methodological uncertainties and data availability) **that need further methodological development** and data gathering efforts. Covering those gaps will allow the industry to go further in its sustainability measurement. Please see the areas of concern and the call to action raised in appendix 11.

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[1] A life cycle assessment (LCA) is a compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle (source: ISO 14040:2006).

2. Introduction

The purpose of this guidance

The objective of the *Life Cycle Metrics for Chemical Products* guidance **is to support the consistent and credible communication of a product's environmental footprint by the chemical sector**. The guidance proposes a global framework to align life cycle metrics to determine the footprint of chemical products based on state-of-the-art LCA developments and methodologies.

The guidance is part of the World Business Council for Sustainable Development's (WBCSD) Reaching Full Potential (RFP) Chemical Sector Project, which aims to develop collaborative solutions from the chemicals value chain towards a sustainable 2050. The RFP Project includes three work streams:

- Life Cycle Metrics: to develop a guide for consistent and credible communication to stakeholders on a chemical product's sustainability impact through its life cycle;
- Avoided Emissions:[2] to develop a guide for consistent and credible communications of emissions avoided through a chemical product's use in the value chain;
- Collaboration in the Value Chain: to identify pre-competitive barriers and solutions to bring existing chemical solutions to market faster-emphasising the long-term disruptors and enablers towards Vision 2050.[3]

This document is part of the Life Cycle Metrics work stream.

How it was developed

The guidance is the result of a collaborative process among 10 global chemical companies that are WBCSD members. It is supported by the European Chemical Industry Council (CEFIC). These companies formed a working group that met over the course of 12 months and cooperatively shared best practices. The outcome, this sector guidance, is designed to improve the harmonisation and consistency of chemical product life cycle assessments.

The working group was chaired by DSM and co-steered by DSM and Solvay. Working group members included AkzoNobel, BASF, Eastman, Evonik, Henkel, Mitsubishi Chemical Holdings, SABIC and SCG Chemicals. The working group was supported by PricewaterhouseCoopers.

The working group also held a stakeholder engagement process to seek feedback on this guidance.

What is the relationship to existing standards and guidelines?

The key feature of this guidance is to go beyond the well-accepted standards for some key topics listed below, by providing additional guidance specific to the chemical industry.

It is built upon existing best practice standards for product environmental footprint assessment (see appendix 10), most notably the International Organization for Standardization's ISO 14040:2006 – "Environmental management – Life cycle assessment – Principles and framework" and ISO 14044:2006– "Environmental management - Life cycle assessment - Requirements and guidelines". Other recognised international guidance, such as the GHG Protocol standards developed by the World Resources Institute (WRI)/WBCSD, the European Commission's *Product Environmental Footprint (PEF)* guide (draft version dated 2013) and other existing sector guidance, were used in the development of this guideline.

This guideline is complementary to international standards on life cycle assessment and environmental footprint and does not intend to replace them. Thus, relevant recommendations or standards, such as ISO 14044:2006 and the PEF Guide, shall be followed to claim alignment with them and with the present guideline.

We rely heavily on WBCSD's **existing guidance documents for the chemical industry** – specifically the *Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain* and *Addressing the Avoided Emissions Challenge* – as they are the results of collaborative processes among the sector and with other external stakeholders and institutions. The GHG Protocol standards are now broadly accepted and applied by the industry for annual corporate reporting.

For more details on the relationship or positioning of this guidance with other standards, please refer to appendix 10, which includes a table comparing the document's requirements with other standards.

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[2] The RFP avoided emissions guidelines are published separately by WBCSD and the International Council of Chemical Associations (ICCA) as *Addressing the Avoided Emissions Challenge* (2013). The report is available at http://www.wbcsd.org/chemicals.aspx.

[3] The WBCSD's cornerstone Vision 2050 report calls for a new agenda for business laying out a pathway to a world in which 9 billion people can live well, and within the planet's resources, by mid-century. More information is available on the WBCSD website: http://www.wbcsd.org/vision2050.aspx.

Who should use this guidance?

This guidance is designed for chemical companies worldwide. It is intended to be used by:

- Chemical companies that seek to assess and communicate the environmental footprint of their products, and especially:
  - For LCA practitioners performing chemical product life cycle assessments and communicating the results to value chain partners;
  - For chemical company stakeholders using LCA results to inform decision-making processes related to business goals.
- Chemical sector value chain stakeholders, in order for them to understand the assumptions supporting the environmental product claims of the chemical sector.

Current guidance scope

This guidance is meant for the calculation of product environmental footprint in an attributional way. Consequential studies, which are useful to assess changes in environmental flows due to decisions, are out of the scope of this guideline. Consequential studies adhere to different principles and therefore would need a guidance of their own.

This guidance is a significant step towards the sustainable assessment of chemical products. It covers the environmental impact assessment and provides clear requirements, notably on:

- Impact categories to be covered when assessing the environmental chemical product footprint and associated impact methods to be used for the assessment;
- Methodological choices to be followed when conducting the assessment;
- Data quality management;
- Key information to be provided when communicating the results of the assessment.

The following topics are not fully covered in this guidance, but may be investigated for later versions

- Environmental metrics:
  - › Toxicity (only partially covered by this guidance due to a large degree of uncertainty in metrics);
  - › Water scarcity (only partially covered by this guidance due to lack of sufficient metrics);
  - › Indirect greenhouse gas (GHG) emissions (not covered in this guidance or in the GHG Protocol standards, but which some LCA practitioners have started to assess).
- Social metrics.

How it will be updated

This guidance is a first approach for the chemical sector towards setting a global methodology for assessing and reporting the life cycle environmental footprint of chemical products along their value chain.

Further challenges may be addressed in future phases of the Life Cycle Metrics project:

- Additional and challenging metrics: notably social impact assessments and further environmental impact categories or metrics where methodological limits were raised during this first phase of the project (e.g., toxicity or water scarcity);
- Sustainability metrics for targeted chemical products categories;
- Additional user-oriented features, such as a checklist for quality assessment, a template for data collection, and/or an extended description of best practices;
- The development of a common knowledge base of relevant information, e.g., literature, contacts, etc.

Call to action

This guidance has been developed by chemical industry companies based on currently available LCA methodologies and developments. However, for some impact categories, further development is needed to properly assess the impact of chemical products and reduce the level of uncertainties, as was clearly emphasised during the project. This especially concerns the following areas:

1. Difficulty in dealing with regional specificities (especially for air acidification, resource depletion, water scarcity and quality, human toxicity and eco-toxicity impact assessment);
2. Difficulty in applying water footprint methods and tools for product assessment;
3. Gaps in human toxicity and eco-toxicity impact assessment methods.

Characterisation factors for many substances are not available or not well established. The high variability of some characterisation factors between different impact assessment methods reveals the uncertainty surrounding the impacts of these materials on the environment and health. Moreover, current inventories from data sets are in some cases highly uncertain, causing additional uncertainty in the assessment of human toxicity and eco-toxicity impacts.

The international scientific community and many other stakeholders from the public and private sector are already working on these issues. However, reaching a consensus on those impact categories would further improve the assessment and communication on the environmental footprint of products. The present working group calls for further discussion with relevant parties to share priorities with the common objective of helping to accelerate the development of more robust methods.

The areas of concern and associated call to action for scientific, LCA database and LCA software development communities are detailed in appendix 11.

How to read this guide

The key requirements of this guidance are presented in coloured boxes to enhance readability.

In addition, relevant examples from the chemical sector, explanations of key concepts and, where relevant, a summary of the main requirements of ISO 14040:2006 and 14044:2006 are also provided.

When this is the case, the reference methodology guide is mentioned in brackets at the end of the quoted requirement.

Requirement status

In order to allow the assessment of the robustness of a chemical product footprint report with regard to this guidance, all requirements from this guidance are marked as either “shall”, “should” or “may” (definitions adapted from the *International Reference Life Cycle Data System (ILCD) Handbook*):

- **SHALL:** mandatory requirement that must always be followed, excluding any specifically named exceptions, if any.
- **SHOULD:** requirement that must be followed. Deviations are permissible if they are clearly justified in writing, giving appropriate details. Reasons for deviation can include a lack of applicability or if another solution is clearly more appropriate.
- **MAY:** a methodological or procedural recommendation. The issue can be ignored or addressed in another way without the need for any justification or explanation.

3. Principles

This guidance adopts the five accounting principles of the *GHG Protocol: Product Life Cycle Accounting and Reporting Standard*: relevance, completeness, consistency, transparency and accuracy. It additionally adopts feasibility as a sixth principle to provide consistency with the *WBCSD's Addressing the Avoided Emissions Challenge (October 2013)*. These principles guide users in the implementation of this document, especially when making choices that are not specified by this guidance document.

Relevance

Ensure the chemical product footprint assessment appropriately reflects the actual input and output flows of the system as much as possible and serves the decision-making needs of users – both internal and external to the company.

Completeness

Account for and report on all energy and emission sources and activities for the given functional unit and within the chosen inventory boundary.

Disclose and justify any specific exclusions.

Consistency

Use consistent methodologies to allow for meaningful comparisons of emissions and energy over time.

Transparently document any changes to the data, inventory boundary, methods, or any other relevant factors in the time series.

Transparency

Address all relevant issues in a factual and coherent manner based on a clear audit trail.

Disclose any relevant assumptions and make appropriate references to the accounting and calculation methodologies and data sources used.

Accuracy

Ensure that the quantification of input and output flows of the system is systematically neither over nor under actual flows, as far as can be judged. Ensure that uncertainties are reduced as far as practicable.

Achieve sufficient accuracy to enable users to make decisions with reasonable assurance as to the integrity of the reported information.

Feasibility

Ensure that the chosen approach can be executed within a reasonable timeframe and with a reasonable level of effort and cost.

4. Life cycle metrics for chemical products footprint

4.1. Compliance with ISO

Chemical product footprint studies **shall** be based on the ISO 14040:2006 and 14044:2006 requirements as much as feasible. All deviations **shall** be explained and documented in the product footprint report.

4.2. Goal and scope definition

A clear definition of the chemical product footprint study goal is critical for alignment between the results and expectations of the study. A clear scope definition focuses the analysis on the intended goal.

Conclusions of the chemical product footprint study **shall** be consistent with the study goal.

In compliance with ISO 14040:2006 and ISO 14044:2006, the following specific requirements are to be taken into account for a chemical product footprint study goal definition. The chemical product footprint study report **shall:**

- State the intended application(s) of the chemical product footprint results in a precise and unambiguous way (*ILCD Handbook*);
- Explain the reasons for carrying out the chemical product footprint study. Name the drivers and motivations and especially identify the decision context (*ILCD Handbook*);
- State the business goal clearly (*GHG Product Protocol*);
- Identify the target audience of the study, i.e., to whom the results of the study are intended to be communicated (*ILCD Handbook*).

Examples of goals of a chemical footprint assessment for the chemical sector:

- Typical examples of intended applications for chemical product footprint studies include the following (see *ILCD Handbook* for more details):
  - **Eco-design and monitoring:** Detailed chemical product eco-design, identification of environmental performance indicators for a specific product, supply chain greening, identifying product groups with the largest environmental improvement potential;
  - **Benchmarking and comparison:** Benchmarking/comparison of specific chemical products, development of eco-label criteria, product category rules, identifying product groups with the largest environmental impact;
  - **Communication:** Development of a life cycle based Type III environmental declaration for a specific good or service;
  - **Policy:** Green public or private procurement, forecasting and analysis of the environmental impact of pervasive technologies, raw material strategies, etc., and related policy development;
  - **Development of specific, average or generic unit process** or life cycle inventory (LCI) result data sets for use in specified types of LCA applications.
- Typical examples of reasons for carrying out the study (including business goal – see GHG Product Protocol for more detail):
  - Answer customer's questions and requests for information;
  - Voluntarily provide information on the product environmental impact (to customers or any other third parties);
  - Optimise or develop new products;
  - Identify new market opportunities and regulatory incentives;
  - Track possible efficiency improvements throughout a product life cycle over time;
  - Supplier and customer stewardship;
  - Enhance employee retention and recruitment resulting from pride in product stewardship.
- Typical examples of intended audience include: internal and/or external stakeholders, such as employees, shareholders, customers, regulators, local communities, society, etc.

4.3. System boundary

4.3.1. Definitions

Cradle-to-grave LCA: Addresses the environmental aspects and potential environmental impacts (e.g., use of resources and the environmental consequences of releases) in a product's life cycle, from raw material acquisition through production, use, end-of-life treatment, recycling and final disposal (ISO 14040:2006 and 14044:2006).

Cradle-to-gate study: Addresses the environmental aspects and potential environmental impacts (e.g., use of resources and the environmental consequences of releases), from raw material acquisition to the point at which it leaves the gate of the factory (i.e., excluding transport to use location, use and end-of-life).

4.3.2. Requirements for chemical product footprint

Chemical product footprint system boundaries **should** be cradle-to-grave.

However, since many products from the chemical industry are intermediates and serve multiple applications, cradle-to-gate boundaries are often needed by value chain partners. When the goal of the study is to supply environmental information on a business-to-business level (providing LCA data to customers for use in environmental product declarations - EPDs), cradle-to-gate studies are acceptable.

Cradle-to-gate studies are also relevant for the comparison of functionally equivalent products on a business-to-business level.

For a cradle-to-gate chemical product footprint, boundaries **shall** include end-of-life for all waste streams generated during the production of the product. Boundaries **should** be set such that all inventory inputs and outputs (except for the studied product) are reduced to elementary flows.

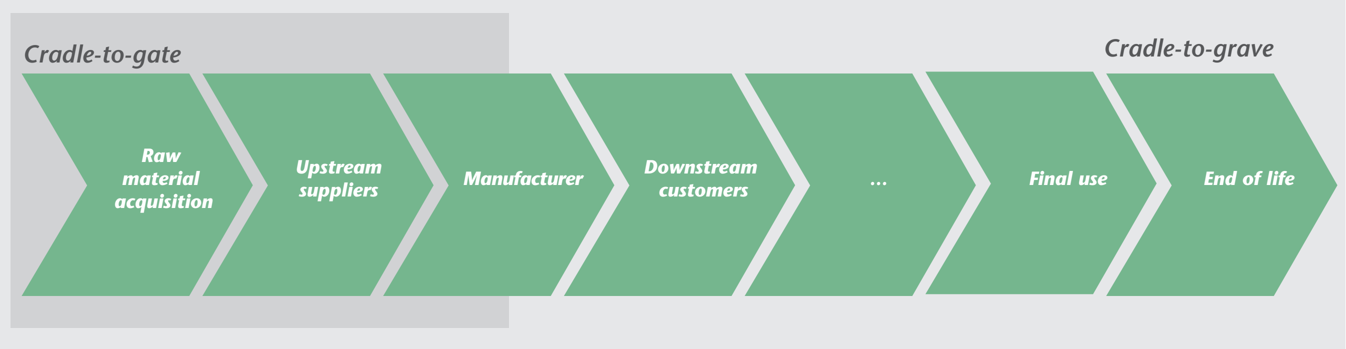

Figure 1: Illustration of cradle-to-grave and cradle-to-gate system boundaries

Cradle-to-gate studies allow for modularity and are most relevant for business-to-business use. Nevertheless, for these studies, differences in chemical product end of life are important to note.

In the case of a cradle-to-gate chemical product footprint study, a specific limitation statement **shall** be included in the chemical product footprint study report in order to inform the reader that comparability of the cradle-to-gate chemical product footprint with other products may not be relevant and might lead to incorrect conclusions because of differences in downstream impacts. For example, GHG emissions generated from the chemical product will be different if the product is landfilled or incinerated at the end of life.

When one or more chemical products are chemically and functionally equivalent in a given application then the cradle-to-gate footprints **may** be compared in a useful way. For example, it may be useful for decision-makers to compare the cradle-to-gate footprints of polypropylene issued from different processes, such as i) the cracking of naphtha or other liquids or ii) the cracking of butane or propane. In such a case, the chemical product footprint life cycle steps taken into account **shall** be clearly listed and described in the chemical product footprint study. Any step exclusion **shall** be justified.

Example of statement that can be used in the chemical product footprint study report:

Please keep in mind that comparisons cannot be made on the level of the product alone. It is necessary to consider the full life cycle of an application to compare the performance of different materials and the effects of relevant life cycle parameters (as in a cradle-to-grave chemical product footprint study). This cradle-to-gate chemical product footprint study is intended to be used by companies to support product-oriented environmental management; by users of the product as a building block of life cycle assessment (LCA) studies of product systems; and by other interested parties, as a source of life cycle information. (Adaptation of PlasticsEurope's Eco-profiles and Environmental Declarations – LCI Methodology PlasticsEurope statement).

Illustrations: Cradle-to-gate or cradle-to-grave?

A cradle-to-gate study is useful in order to substitute an LCI in the value chain of the product (modularity). Hence, cradle-to-gate data can only be used in order to compare products after a complete assessment of the comparability of the downstream environmental impacts of the products. In particular, this impact assessment has to take into account recycling impacts and biogenic emissions (see parts 5.2.2 and 5.2.4).

Case 1: Polypropylene is used in a large variety of industrial applications, such as automotive and packaging. For a given application, it is possible that one or more polypropylene products may be used in an interchangeable way and can be considered to have identical downstream environmental impacts. In that case, it can be relevant to compare the upstream impacts of polypropylene using cradle-to-gate boundaries. These types of analyses are often recommended to benchmark differences in process efficiencies between two products having the same function and fitness-for-use.

Case 2: Xylene is only used in a limited amount of industrial applications, such as solvent, and as a main precursor of terephthalic acid. Since downstream use of xylene is strongly related to the type of product, gate-to-grave impacts of the xylene can vary depending on the producer. In this case, the comparison of upstream impacts of xylene using cradle-to-gate chemical product environmental analysis may lead to the wrong conclusions. Hence, it is preferable to provide external users with the best estimate possible of the full cradle-to-grave environmental impacts.

4.4. Functional unit and reference flow

4.4.1. Definitions

Functional unit: "Quantified performance of a product system for use as a reference unit" (ISO 14040:2006 and 14044:2006).

Reference flow: "Amount of product on which the results of the study are based" (GHG Product Protocol).

4.4.2. Requirements for chemical product footprint

The following requirements have to be taken into account when defining the functional unit (adapted from *Addressing the Avoided Emissions Challenge*):

The functional unit **shall** be consistent with the goal and scope of the study.

As the functional unit specifies the benefit provided to the customer, the functional unit **shall** be equivalent for all compared solutions.

To ensure products in a comparative chemical product footprint study are exchangeable in the selected market, relevant quality criteria **shall** be taken into consideration.

The following three quality properties **shall** be used to assess whether compared solutions are truly exchangeable:

1. Functionality, related to the main function of the solution;

2. Technical quality, such as stability, durability, ease of maintenance;

3. Additional functions rendered during use and disposal.

For cradle-to-grave studies, companies **shall** specify the duration of the functional unit, i.e., how long does the performance of the final product or service need to be maintained. The chemical product footprint report **shall** explain how this duration has been determined in relation to the lifetime of the product.

Both the duration of the functional unit and the lifetime of the product **should** be in line with standards used in the market (e.g., product category rules, studies from reputable organisations and studies by leading companies in the value chain).

Frequent errors to avoid when defining the functional unit of a chemical product footprint:

- Partial definition of a functional unit: For example, in the case of a paint product, the functional unit could be that the paint must cover a 1 m^2 wall and keep its colour quality for eight years. This indicates two functions: wall coverage and colour quality. In that case, omitting one of the criteria may lead the reader to the wrong conclusions.
- Difference between reference flow and functional unit for a cradle-to-gate chemical product footprint: “1 kg of polypropylene” is a flow reference while “producing 1 kg of polypropylene meeting certain sales specifications in [location] in [year of reference]” is a functional unit.

4.5. Impact categories, energy and other flows

4.5.1. Impact category methods for characterisation

The table below lists two levels of requirements:

- Requirement on impact category indicators to be included in the chemical product footprint report (horizontal colored rows)
- Requirement on the characterization models and sources to be used when including an impact category indicator in the chemical product footprint report (column “Guidance requirement for characterization model and source”).

The choice of the impact categories to communicate is supported by the decision tree in appendix 4: Decision tree on the impact categories to communicate, based on the relevance of impact categories to stakeholders, the existence of a global consensus for impact assessment, and data availability.

Impact category	Guidance requirement for characterisation model and source	Characterisation modes	Source	Impact category indicator
The following impact categories SHALL be included in the chemical product footprint report				
Global warming	Specified characterisation model and source shall be used in chemical product footprint study report.	Global warming potential-Infrared radiative forcing (100 year).	Intergovernmental Panel on Climate Change 2007.	kg CO_2 eq.
Photochemical ozone formation	Specified characterisation model and source should be used (local and more appropriate method may be used).	LOTOS-EUROS, except for Japan: LIME 2 Model.	Van Zelm et al. 2008 as applied in ReCiPe. Itsubo, N., A. Inaba 2012, as applied in LIME 2.	kg Ethylene eq.
Air acidification	Specified characterisation model and source may be used (local and more appropriate method may also be used).	Accumulated exceedance model, except for Japan: LIME 2 Model.	Seppälä et al. 2006, Posch et al. 2008. Itsubo, N., A. Inaba 2012, as applied in LIME 2.	mol H+ eq.
Resource depletion (fossil fuels)	Specified characterisation model and source should be used. Specific requirements for energy flows are detailed in section 4.5.2.1	CML 2002 model, except for Japan: LIME 2 Model.	Van Oers et al. 2002. Itsubo, N., A. Inaba 2012, as applied in LIME 2.	kg Sb eq.
Abiotic depletion (element)	Specified characterisation model and source should be used. If the specified characterisation model is applied, a sensitivity analysis on economic and ultimate reserves should be performed.	CML 2002 model, except for Japan: LIME 2 Model.	Van Oers et al. 2002. Itsubo, N., A. Inaba 2012 as applied in LIME 2.	kg Sb eq.
Eutrophication (freshwater)	Specified characterisation model and source should be used (local and more appropriate method may be used).	EUTREND Model, except for Japan: LIME 2 model.	Struijs et al. 2009, as implemented in ReCiPe. Itsubo, N., A. Inaba 2012, as applied in LIME 2.	kg P eq.
Eutrophication (marine)	Specified characterisation model and source should be used (local and more appropriate method may be used).	EUTREND Model, except for Japan: LIME 2 model.	Struijs et al. 2009, as implemented in ReCiPe. Itsubo, N., A. Inaba 2012, as applied in LIME 2.	kg N eq.
Human toxicity and ecotoxicity	Specified characterisation model and source may be used.	USEtox Model.	Rosenbaum et al. 2008.	CTUh (Comparative Toxic Unit for humans) and CTUe (Comparative Toxic Unit for ecosystems)

Impact category	Guidance requirement for characterisation model and source	Characterisation modes	Source	Impact category indicator
The following impact categories SHOULD be included in the chemical product footprint report				
Dust & particulate matter	When this impact category is included in the chemical product footprint report, specified characterisation model and source should be used.	Riskpoll Model.	Humbert 2009.	kg PM2.5 eq.
Land use	When this impact category is included in the chemical product footprint report, specified characterisation model and source may be used. Specific requirements for land occupation flow are detailed in section 4.2.5.3.	Model based on soil organic matter (SOM).	Milà i Canals et al. 2007.	kg C*yr
Species richness	When this impact category is included in the chemical product footprint report, specified characterisation model and source should be used.	ReCiPe (endpoint) or model based on Koellner (2008).	Koellner et al. 2008.	m^2*yr
The following impact categories MAY be included in the chemical product footprint report				
Ozone depletion	When this impact category is included in the chemical product footprint report, specified characterisation model and source should be used.	World Meteorological Organization over an infinite time horizon (as implemented in EDIP and LIME 2).	World Meteorological Organization 2003.	kg CFC-11 eq.
Water scarcity / water availability footprint	When this impact category is included in the chemical product footprint report, specified characterisation model and source should be used. Specific requirements for water consumption flow and water availability footprint are detailed in section 4.5.2.2.	Model based on Pfister (2009) or Global Water Stress Index.	Pfister et al. 2009; WBCSD Global Water Tool; Annual Renewable Water Supply per person database, WRI 1995; Aqueduct's baseline water stress, WRI, 2013.	m^3 eq.

Table 1: Required impact category indicators, characterisation models and sources for chemical product footprint studies

All recommended impact category indicators, characterisation models and sources are compliant with 2013 European Union's Product Environmental Footprint (EU PEF) recommendations, except:

1. World Meteorological Organization (WMO) characterisation source year, which has been updated;
2. Kg ethylene equivalent impact category indicator for photochemical ozone formation has been specified instead of kg non-methane volatile organic compounds (NMVOC) equivalent since kg NMVOC could result in addition of gases with different characterisation factors;
3. The above mentioned impact categories for which regional specificities have a high impact and for which the Lime 2 Model is recommended for Japan;
4. Pfister method for water scarcity, which is more recent than the Frischknecht method recommended in the EU PEF;
5. Species richness has been integrated (and is not part of the EU PEF requirements).

When a characterisation factor is not available for specific substances or emissions flows, please refer to the proxy data section of this guidance (4.6.1.2).

4.5.2. Energy and other flows

4.5.2.1. Energy

The following energy flows **shall** be assessed and reported in the chemical product footprint study report according to the definitions provided below:

- Cumulative energy demand (in MJ);
- Renewable energy consumption (in MJ);
- Non-renewable energy consumption (in MJ).

Cumulative energy demand and renewable/non-renewable energy consumption **shall** be assessed using the lower heating values (LHV) for fuels, also commonly called the net calorific value.

Definitions of energy flows:

- **Cumulative energy demand (CED)**: The CED of a product represents the direct and indirect primary energy use throughout the product system, including the energy consumed during the extraction, manufacturing, disposal of the raw and auxiliary materials (VDI[4]) and product use. CED includes both renewable and non-renewable energy consumption.
- **Renewable energy consumption:** Renewable sources of energy include wind power (both onshore and offshore), solar power (thermal and photovoltaic), hydroelectric power, tidal power, geothermal energy and biomass (including biofuels, bioliquids and waste from biomass). Peat and biomass from primary forests are considered non-renewable (*ILCD Handbook*).
- **Non-renewable energy consumption**: Non-renewable sources of energy include fossil and nuclear energy. Non-renewable energy consumption represents differences between CED and renewable energy consumption.

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[4] VDI 1997. *Cumulative Energy Demand - Terms, Definitions, Methods of Calculation.* VDI-Richtlinien 4600. Düsseldorf: Verein Deutscher Ingenieure.

4.5.2.2. Water consumption

This guidance recognises that water scarcity[5] assessment is under development. The intention of reporting water consumption is a placeholder until more advanced impact assessment methods are feasible and widely available.

Water consumption of the entire system **should** be reported.

When water consumption is reported, the chemical footprint report **shall** include at least cradle-to-gate water consumption according to the following categories:

- Surface freshwater;
- Renewable groundwater;
- Non-renewable (fossil/deep) groundwater.

Renewable groundwater drainage basin **shall** be used only when this has been confirmed by a specific analysis. A renewable groundwater drainage basin is defined as:

"A water drainage basin where average quantity of water storage is either stable or increasing over the years."

Otherwise, groundwater **shall** be defined by default as "non-renewable (fossil/deep) groundwater".

In addition, cradle-to-gate water consumption of seawater **should** also be reported.

The sum of all consumption from these drainage basins **should** cover all water consumption for the chemical product production (see section on cut-off, 5.1.3).

If water consumption is reported, then its scope **shall** also be reported.

Water consumption assessment for an industrial site:

Water consumption from an industrial site **should** be assessed according to the following formula and definitions:

Gate-to-gate water consumption from production site(s) = production site(s) water withdrawal - production site(s) water release to the same drainage basin from which water was withdrawn.

Therefore, water taken from groundwater and released to a river in the same drainage basin, is not considered water consumption but may be reported separately. Losses may be due, for example, to evaporation or incorporation of water into a product or waste.

Definitions:

1. Water withdrawal: Anthropogenic removal of water from any water body or from any drainage basin either permanently or temporarily (based on discussions on draft ISO 14046).
2. Drainage basin: Area from which direct surface run-off from precipitation drains by gravity into a stream or other water body (based on discussions on draft ISO 14046).

When water consumption is reported:

A quantitative assessment based on Pfister et al. (2009) or from a credible water scarcity database or tool, such as the latest version of the WBCSD Global Water Tool, **should** be reported with the following information:

1. Quantity or share of water consumption for which water scarcity has been quantitatively assessed. It **should** correspond to at least the gate-to-gate water consumption.
2. Quantity or share of water consumption by range of water stress index.
3. Reference of the water scarcity database: when using the WBCSD Global Water Tool, the Annual Renewable Water Supply per person database (WRI 1995) or the Aqueduct's baseline water stress (WRI 2013) **may** be used.

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[5] Water scarcity assesses the health of a river system by evaluating the amount of water available within a given area. Scarcity describes the total supply in an area minus a specific type of demand called consumptive use (source: WRI). Water scarcity is defined as the extent to which demand for water compares to the replenishment of water in an area, e.g., a drainage basin, without taking into account the quality (based on discussions on draft ISO 14046). Water scarcity can broadly be understood as the lack of access to adequate quantities of water for human and environmental uses (Source: Global Water Forum).

See below the split of water consumption by ranges of Baseline Water Stress Indexes for a total water consumption of 310 L per functional unit as an example:

Unit: WRI Aqueduct tool Baseline water stress raw value	Extreme scarcity risk >80%	High scarcity risk 40% to 80%	Medium to high scarcity risk 20% to 40%	Low to medium scarcity risk 10% to 20%	Low risk < 10%	Arid and low water use	No water scarcity assessment available
For a total water consumption of 310 litres per functional unit	100 litres	0 litres	0 litres	200 litres	0 litres	0 litres	10 litres

Table 2: *Split of water consumption by ranges of Baseline Water Stress Indexes*

The WRI Aqueduct tool is available at http://www.wri.org/our-work/project/aqueduct/aqueduct-atlas.

The WBCSD Global Water tool is available at http://www.wbcsd.org/work-program/sector-projects/water/global-water-tool.aspx.

4.5.2.3. Land occupation

Land occupation intermediary flow **may** be assessed and disclosed in the chemical product environmental footprint. If disclosed, this indicator **should** be accounted in m²a unit (area in square meters*year).

The following land categories **may** be used for classification (source: ecoinvent):

- occupation, urban
- occupation, industrial area
- occupation, traffic area
- occupation, mineral extraction site
- occupation, dump site
- occupation, arable
- occupation, arable, monotone-intensive
- occupation, arable, non-irrigated organic
- occupation, permanent crop
- occupation, pasture and meadow
- occupation, forest
- occupation, shrub land
- occupation, water areas

Land transformation (m²) **may** be considered as well for reporting.

The soil organic matter land-use impacts (in kg C*yr) described in section 4.5.1 differ from the land occupation flows (in m²a). A holistic assessment of land-use impact could consider land-occupation flows, land-use changes and specific characterisation factors taking into account species richness impacts of land usage.

4.5.2.4. Waste

Wastes are intermediary flows in a product system, exchanged between the unit process that generates them and the one(s) that treat them. Accounting for them **should** not prevent the practitioner from including the treatment process and the associated burdens since these are part of the cradle-to-grave life cycle and cradle-to-gate life cycle for the product system.

For cradle-to-gate studies:

- The waste tonnages **may** be disclosed according to the following categories:
- Hazardous waste disposed
- Non-hazardous waste disposed
- Radioactive waste disposed

When waste flows are disclosed, all types of disposed waste (landfill and incineration without energy recovery) **should** be accounted for.

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[7] The conditions of EU Directive 2008/98/EC for incineration with energy recovery specify that energy efficiency must be up to 60% or 65%. These include incineration facilities dedicated to the processing of municipal solid waste only where their energy efficiency is equal to or above:

- 60% for installations in operation and permitted in accordance with applicable community legislation before 1 January 2009;
- 65% for installations permitted after 31 December 2008 (EU Directive 2008/98/EC, p.24).

4.5.3. Non LCI information

There are sources of information outside of environmental chemical product footprints that provide quantitative or qualitative data for product safety and toxicity communication. Therefore, other relevant information **may** be included in the chemical product footprint report, such as extracts from:

- Safety data sheets (SDS) that provide information on health, safety, environment and transportation;
- GreenScreen®;
- Inclusion/exclusion on regulatory (e.g., REACH – Registration, Evaluation, Authorization and Restriction of Chemicals) or non-regulatory lists.

4.6 Data source requirements and quality management

4.6.1 Primary and secondary data requirements

Definitions

Primary data: Data from specific operations in the studied product's life cycle (*GHG Product Protocol*) that is measured.

Secondary data: Process data that is not from specific processes in the studied product's life cycle (*GHG Product Protocol*).

The quality of all data **shall** be assessed according to the criteria specified in section 5.1.2.

4.6.1.1. Primary data

The most accurate and available primary data **shall** be used. Any use of secondary data when primary data is available **shall** be justified using the pedigree matrix (see section 5.1.2.1).

Requirements regarding secondary data sources are detailed in section 5.1.1.1.

The most accurate available data **shall** be used for *primary data*.

The following on-site measurements **should** be used in priority when data is available and accurate:

- Aggregation of registered measures for consumptions (water, energy, raw material);
- Continual measurements for air and water emissions (if not available, spot measurements may be used).

Detailed examples of specific data sources are provided in chapter 5.7 *Specific data collection*, page 55 of the *EU Product Environmental Footprint Guide*.

The case of electricity:

The electricity grid mix **should** be selected based on the goal of the LCA. For example, if the LCA goal is to compare the industry average impact of chemicals, a country or global average or industry average electricity mix should be used. However, if the LCA goal is to compare across specific plants or the chemicals produced in specific locations, supplier-specific electricity should be used.

The following recommendations adapted from and in line with the European PEF **shall** be applied for electricity:

Supplier-specific data **shall** be used if available when the goal is to assess specific (not average) production systems. A statement of the supplier **shall** then be included as an annex to the chemical product footprint report, validating that the electricity supplied is effectively generated using renewable sources and is not sold to any other organisation.

If supplier-specific data is not available or if the goal is to assess average production systems, then country-specific consumption-mix data **shall** be used for the country in which the life cycle stages occur.

There **should** not be any double counting of renewable electricity (and associated impacts) between renewable energy produced within the chemical product production plant boundary and the grid energy consumed upstream.

If no data is available on the calculation of corrected mixes, the uncorrected average mixes **shall** be used. It **shall** be transparently reported which energy mixes are assumed for the calculation of the benefits and whether or not these have been corrected.

4.6.1.2. Secondary data

Quality of secondary data (including supplier data) **shall** be assessed according to the criteria specified in section 5.1.2.

The sources of secondary data to be used **should** be based on the quality assessment results from the following list of source categories:

1. LCI data sets from recognised sources:
   - 1.1. Industry average eco-profiles published by associations or federations (when consistent with the goal of the chemical product footprint study);
   - 1.2. Results of LCA studies published in the literature (only when consistent with the goal of the chemical product footprint study);
   - 1.3. Generic databases.
2. Proxy data;
3. Technical literature.

The above list **may** also be used as an order of choice for the default selection of secondary data that are not critical to the product footprint assessment results.

For all secondary data, specific attention has to be paid to the choices and methodology underlying these data sets. The inherent assumptions **shall** be carefully considered by the practitioner before using the data. Allocation approaches used (if any), cut-off, data gaps (lack of or incomplete emissions data, etc.) **should** be reported.

Further detailed specifications for each type of secondary sources are detailed below.

Further information on secondary data and generic source is provided in appendix 5 and appendix 6.

Source 1.1: Industry average eco-profiles published by associations or federations

Specific attention **shall** be paid to the assumptions regarding the allocation of material recycling within the life cycle in all databases.

Source 1.2: Results of LCA studies published in the literature

LCA study literature can be used. Data from peer-reviewed sources is preferred over non-peer-reviewed sources. Only results with clear methodological assumptions that are investigated and challenged **should** be used as secondary data.

Examples of sources:

- *International Journal of LCA;*
- Published environmental product declaration (EPD) (e.g., www.environdec.com);
- LCA published by chemical products producers and compliant with ISO 14040:2006 and 14044:2006 standards.

Source 1.3: Generic databases

See appendix 5 for more guidance on generic databases.

Source 2: Proxy data

When there is no LCI data set corresponding to a specific process or input, proxy data can be used to estimate the impact of this input. In that case, the most representative (similar production processes) and conservative LCI data set available within the sources can be chosen to estimate or extrapolate the impact. Especially for a particular chemical or product, proxy data sets **should** be selected based on “substitute” data sets for products produced using the same/similar value chain and/or similar technology to ensure their cradle-to-gate stories are comparable.

The hypothesis and reasons for selecting these proxy data **shall** be explained and detailed within the chemical product footprint report.

Example of ethane proxy data:

If a data set on ethane is not available, appropriate data sets for propane or butane (which are also co-produced from natural gas) can be used. Ethylene is not an appropriate substitute as this chemical does not carry similar life cycle burdens because it requires a different production route.

Source 3: Technical literature

When no sufficiently representative data set is found in previously listed data sources, the modelling **may** be performed using literature data and/or theoretical calculation. Bibliographical sources **shall** be reported in the chemical product footprint report.

4.6.2. Data quality management

4.6.2.1. Data quality indicators

Data quality indicators:

The following five indicators **should** be used to assess the quality of the data (both primary and secondary) used for the modelling:

- Reliability or parameter uncertainty;
- Completeness;
- Time representativeness;
- Geographical representativeness;
- Technological representativeness.

Scoring:

The data quality scoring **should** be assessed according to data quality ratings from EU PEF. The table reproduced below describes the quality level scoring (from 1 to 5, with 1 representing the highest score and 5 representing the lowest score) for each criterion. The assessment and rating on data quality **should** be performed for each unit process with a significant contribution (>10 percent) to at least one environmental impact. The results **should** then be aggregated at the life cycle stage level.

Further guidance on assessing uncertainty factors is available in the EU PEF (section 5.6 on data quality requirements).

The pedigree matrix (from ecoinvent database version 3 data quality guidelines, Weidema et al. 2013) provides further guidance on reliability, time, geographical and technological representativeness and therefore may also be used in data quality assessment.

Indicator score	1	2	3	4	5 (default)
Definition	Meets the criterion to a very high degree, without need for improvement	Meets the criterion to a high degree, with little significant need for improvement	Meets the criterion to an acceptable degree, but merits improvement	Does not meet the criterion to a sufficient degree. Requires improvement	Does not meet the criterion. Substantial improvement is necessary. OR: This criterion was not judged / reviewed or its quality could not be verified / is unknown
Completeness (EU PEF)	Very good completeness (≥90%)	Good completeness (80% to 90%)	Fair completeness (70% to 80%)	Poor completeness (50% to 70%)	Very poor or unknown completeness (<50%)
Time representativeness (EU PEF)			Context specific		
Geographical representativeness (EU PEF)			Context specific		
Technological representativeness (EU PEF)			Context specific		
Completeness (EU PEF)	Very low uncertainty (≤ 10%)	Low uncertainty (10% to 20%)	Fair uncertainty (20% to 30%)	High uncertainty (30% to 50%)	Very high uncertainty (> 50%)
Temporal correlation (Pedigree matrix)	Less than 3 years of difference to the time period of the dataset	Less than 6 years of difference to the time period of the dataset	Less than 10 years of difference to the time period of the dataset	Less than 15 years of difference to the time period of the dataset	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical correlation (Pedigree matrix)	Data from area under study	Average data from lager area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown or distinctly different area (North America instead of Middle East, OECD-Europe instead of Russia)
Further technological correlation (Pedigree matrix)	Data from enterprises, processes and materials under study	Data from processes and materials under study (i.e. identical technology) but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes and materials	Data on related processes on laboratory scale or from different technology
Reliability (Pedigree matrix)	Verified* data based on measurements**	Verified data partly based on assumptions or non-verified data based on measurements	Non- verified data partly based on qualified estimates	Qualified estimates (e.g. by industrial expert)	Non-qualified estimate

Table 3: Data quality rating – adapted from EU PEF and Pedigree matrix

[*] Verification may take place in several ways, e.g., by on-site checking, by recalculation, through mass balances or cross-checks with other sources.

[**] Includes calculated data (e.g., emissions calculated from inputs to an activity) when the basis for calculation is measurements (e.g., measured inputs). If the calculation is based partly on assumptions, the score would be 2 or 3.

4.6.2.2. Data management plan

A data management plan documents the product inventory process and the internal quality assurance and quality control procedures in place to enable the preparation of the life cycle inventory from its inception through its final reporting. The data used for chemical product footprint **shall** be managed according to the GHG Product Protocol "Data Management Plan Checklist" (see Appendix 9).

Moreover, the chemical product footprint report is responsible for ensuring the applicability of the information to meet users' needs. Chemical product footprint studies **should** include a statement for users to periodically check if the chemical product footprint is valid over time and indicate where updated necessary information will be available.

4.6.3. Cut-off

Environmental significance **shall** be assessed as defined by ISO 14040:2006 and 14044:2006 based on expected emissions. See example below for materiality of toxic material flows.

All mass and energy elementary flows **should** be accounted for. If not, the chemical product footprint study report **shall** include the estimation of completeness, based on:

- Mass cut-off (in percent of total system input mass): Best estimation of the mass of all non-accounted components of the product.
- Energy cut-off (in percent of total energy consumption): Estimation of all energy consumption (cumulative energy demand) of non-accounted mass inputs.

Examples of cut-off:
Hazard communication information, such as a safety data sheet, can allow for the identification of compounds with potential risk for toxicity or other safety concerns.

Example 1: A water-repellent product

A water-repellent coating contains 0.01% (mass) of a fluorocarbon material (responsible for the repellent effect). Using the mass cut-off for this raw material could lead the user to not model this raw material. Nevertheless, this fluorocarbon product is classified on the safety datasheet as a severe acute toxin for dermal contact. Hence, it is critical to include this fluorocarbon material in order to assess the toxicity impacts of the water repellent. This example demonstrates the benefit of using easily available safety data sheet (SDS) classifications for cut-off decisions.

Example 2: Inclusion of palladium (fine chemical production)

The amount of input palladium intermediate for the catalyst step for the production of a chemical product weighs only 0.01 grams per kilogram of product. Nevertheless, it accounts for 28 percent of the global warming impact and 98 percent of the acidification impact. This example shows the importance of taking all intermediates into account, even though its mass significance is very low.

Unless they are expected to be material, the following elements **should** be excluded from the scope of the chemical product footprint study:

- Business travel (according to the GHG Protocol scope 3 definition);
- Employee commuting (according to the GHG Protocol scope 3 definition);
- Investments (according to the GHG Protocol scope 3 definition);
- Infrastructure life cycle impacts;
- Energy consumption and goods not directly related to the product's production; for example recreation facilities, canteen, administration and R&D-related impacts.

In case it is not feasible to apply these exclusions (in particular, if data sets do not allow it), a statement **should** be included in the data quality section of the chemical product footprint report.

4.7. Main methodological choices

4.7.1. Allocation rules between co-products

4.7.1.1. Key concepts

Key allocation concepts from ISO 14040:2006 and 14044:2006 standards are summarised below:

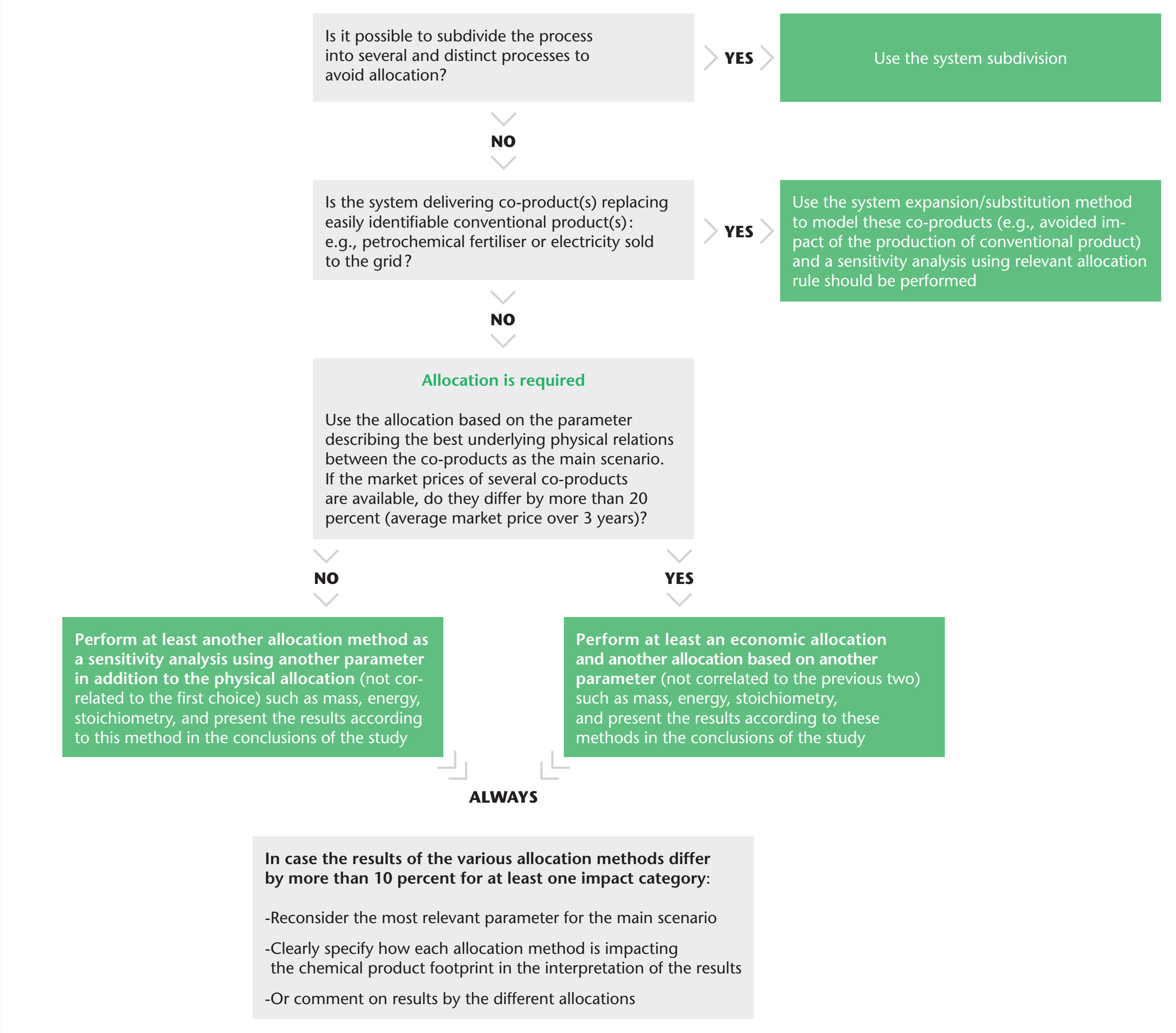
- › **System subdivision:** Dividing the unit process to be attributed into two or more sub-processes and collecting the input and output data related to these sub-processes.
- › **System expansion/substitution:** Expanding the product system to include the additional functions related to the co-products.
- › **Physical relationships allocation based notably on mass, energy and stoichiometry parameters:** The inputs and outputs of the system are partitioned between its different products or functions in a way that reflects the underlying physical relationships between them, i.e., they should reflect the way in which the inputs and outputs are changed by quantitative changes in the products or functions delivered by the system.

  Economic allocation: Input and output data are allocated between co-products in proportion to the economic value of the products.

4.7.1.2. Allocations rules

When a system delivers more than one product with different functions, the following decision tree **should** be used to choose the method to allocate the environmental impacts of each product.

Allocation rules decision tree[9]



Is it possible to subdivide the process into several and distinct processes to avoid allocation?

Use the system subdivision

Is the system delivering co-product(s) replacing easily identifiable conventional product(s): e.g., petrochemical fertiliser or electricity sold to the grid?

Use the system expansion/substitution method to model these co-products (e.g., avoided impact of the production of conventional product) and a sensitivity analysis using relevant allocation rule should be performed

Allocation is required

Use the allocation based on the parameter describing the best underlying physical relations between the co-products as the main scenario. If the market prices of several co-products are available, do they differ by more than 20 percent (average market price over 3 years)?

Perform at least another allocation method as a sensitivity analysis using another parameter in addition to the physical allocation (not correlated to the first choice) such as mass, energy, stoichiometry, and present the results according to this method in the conclusions of the study

Perform at least an economic allocation and another allocation based on another parameter (not correlated to the previous two) such as mass, energy, stoichiometry, and present the results according to these methods in the conclusions of the study

In case the results of the various allocation methods differ by more than 10 percent for at least one impact category:

-Reconsider the most relevant parameter for the main scenario

-Clearly specify how each allocation method is impacting the chemical product footprint in the interpretation of the results

-Or comment on results by the different allocations

Figure 2: Allocation rules decision tree

Examples for allocations are detailed in Appendix 7.

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[9] The 20 percent rule for market prices is based on the recommendations from the Accounting and Reporting Corporate GHG Emissions in the Chemical Sector guide. This value is used to perform allocations in cases where market prices differ significantly between co-products.

4.7.2. Attribution of recycling benefits

When a consensus along a value chain has already defined a specific allocation method (i.e., corrugated board, steel, aluminium, and *industry average eco-profiles published by industry associations*) the consensus attribution method **should** be used.

In other cases, recycling **should** be accounted as described in the EU PEF using the 50/50 attribution method: “the formula provided […] allocates impacts and benefits due to recycling equally between the producer using recycled material and the producer producing a recycled product: 50/50 allocation split” (EU PEF)[10].

Whatever the choices made on the attribution of recycling impacts/benefit:

The results **shall** be communicated both with the total amount of impacts and including the recycling credit attribution.

A sensitivity analysis **shall** be performed using the EU PEF 50/50 method.

An illustration for the recycling of a polyethylene terephthalate (PET) bottle is presented in Appendix 8.

4.7.3. Avoided emissions

When comparing alternative solutions within the chemical industry value chain, avoided emissions **shall** be accounted for and attributed as specified in the WBCSD’s *Addressing the Avoided Emissions Challenge*, October 2013.

4.7.4. Bio-based carbon storage

Separate accounting and reporting shall be performed for fossil and bio-based carbon emissions and the carbon stored in the raw biomass shall also be quantified.

In a cradle-to-gate study, a carbon credit appears as a negative value due to CO_2eq uptake during the growing phase of the plant at the origin of the renewable material.

The fate of this bio-based carbon content in the product depends on the end-of-life of the final product and therefore often leads to a neutral balance due to the release of the bio-based carbon at the end-of-life (in case of incineration for instance).

In such cases, the end-of-life of the product and its impact on the carbon elementary flow balance shall be at least qualitatively described in the chemical product footprint report.

4.7.5. Carbon storage and delayed emissions

The sensitivity of GHG emissions and removals associated with temporary carbon storage or delayed emissions **should** be assessed, and therefore the sensitivity **should** be discussed when interpreting the global warming impact results.

When being communicated, carbon delayed emissions **shall** be reported separately.

For more information on temporary carbon storage and the way to assess delayed emissions, please refer to ISO/TS 14067:2013.

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[10] This approach is based on the open loop system where the market shows no visible disequilibrium (allocation 50/50) and is also recommended in closed loop systems.

4.7.6. Direct land-use change/indirect land-use change

Greenhouse gas emissions that occur as a result of indirect land-use change **should** not be considered.

Greenhouse gas emissions from direct land-use change **shall** be allocated to goods or services for 20 years[11] after the change occurs using the Intergovernmental Panel on Climate Change (IPCC) default values table below (IPCC updates of this table should be preferably used, if available):

Blome	**Area**		**Global carbon stack (GT C)**	
	(10^9 ha)	Vegetation	Soil	Total
Tropical forests	1.76	212	216	428
Temperate forests	1.04	59	100	159
Boreal forests	1.37	88	471	559
Tropical savannas	2.25	66	264	330
Temperate grasslands	1.25	9	295	304
Deserts and semi-deserts	4.55	8	191	199
Tundra	0.95	6	121	127
Wetlands	0.35	15	225	240
Croplands	1.60	3	128	131
Total	**15.12**	**466**	**2,011**	**2,477**

Note: Global carbon stocks in Gt C shall be converted to Gt CO_2 eq. by multiplying by the stoichiometric factor 11/3.

Table 4: IPCC default values for greenhouse gas emissions

For a product produced within 20 years after the land-use change occurs, changes in carbon stocks shall be allocated for the product using the following formula:

$$\textbf{Greenhouse gas emissions per product } (GT\ CO_2\ eq./unit)$$

$$= \frac{[\textbf{Area occupied by the factory ha}] \text{ X } [\textbf{Total IPCC Carbon Stock } (GT\ C)] \text{ X } [CO_2 \textbf{Conversion factor } (GT\ CO_2\ eq./GT\ C)]}{[\textbf{IPCC default land area ha}] \text{ X } [\textbf{Numberof years after land change years}] \text{ X } [\textbf{Yearly production } (units/year)]}$$

When the product is produced more than 20 years after the land-use change has occurred, no further change in carbon stock is considered.

Example of greenhouse gas emissions from direct land-use change calculations:

A factory producing only product X occupies 2 hectares and produces an average of 1 million units of product X per year.

The product is produced during the 20 years succeeding the land-use change. Before the factory was built, the land was a tropical forest. The greenhouse gas emissions from direct land-use change are calculated according to the following formula and gives the following results:

$$\textbf{Greenhouse gas emissions per product } (GT\ CO_2\ eq./unit)$$

$$= \frac{\text{(2 [Area occupied by the factory in ha] x 428 [Total IPCC Carbon Stock for tropical forests in GT C] x 44/12 [} CO_2 \text{ conversion factor in GT } CO_2\ eq./GT\ C\text{])}}{\text{(1,76*}10^9\text{ [IPCC default land area for tropical forests in ha] x 20 [Number of years after land change year] x 1 000 000 [Yearly production in units/year])}}$$

$$= 8{,}92 \text{ x } 10^{-14}\ GT\ CO_2\ eq./unit$$

$$= 8{,}92 \text{ x } 10^{-2}\ kg\ CO_2\ eq./unit$$

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[11] The use of 20 years as a threshold is consistent with the defaults contained in the IPCC *Special Report on Land Use, Land Use Change and Forestry* (2000).

4.8. Uncertainties of results

At least a qualitative description of uncertainties **shall** be provided (EU PEF).

Quantitative uncertainty assessments **may** be calculated for variance associated with significant processes and characterisation factors using Monte Carlo simulations.

See ILCD recommendations for more details on how to assess uncertainties.

4.9. Critical/peer review

Peer review of chemical product footprint study reports **shall** be conducted to assess consistency with this guidance. In the case of external publication of comparative assertions, an external critical review by a panel of LCA experts **shall** be performed prior to publication in accordance with ISO 14040:2006 and 14044:2006. If the comparative study is internal, the critical review **shall** be performed at least internally.

If the chemical product footprint report does not include comparative assertions, an internal critical review **shall** be performed according to the same requisites as for an external review.

A chemical product footprint study report shall include a statement clearly specifying that the study has been critically/peer reviewed and summarising the conclusions of that review.

Appendices

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2. Terminology

attributional: Refers to process-based modelling intended to provide a static representation of average conditions, excluding market-mediated effects.

chemical product footprint: Multi-criteria measure of the environmental performance of a chemical product throughout its life cycle.

comparative assertion: Claim regarding the superiority or equivalence of one product or solution versus a competitor's product that performs the same function (definition based on ISO 14045 and does not interpret, change or subtract from the requirements of ISO 14044:2006).

cradle-to-gate study: Addresses the environmental aspects and potential environmental impacts (e.g., use of resources and the environmental consequences of releases), from raw material acquisition to the point at which it leaves the gate of the factory (i.e., excluding transport to use location, use and end-of-life).

cradle-to-grave LCA: Addresses the environmental aspects and potential environmental impacts (e.g., use of resources and the environmental consequences of releases) in a product's life cycle, from raw material acquisition through production, use, end-of-life treatment, recycling and final disposal (source: ISO 14040:2006 and 14044:2006).

comparative chemical product footprint study: Chemical product footprint study including comparative assertions about chemical products.

cumulative energy demand (CED): Represents the direct and indirect primary energy use throughout the product system, including the energy consumed during the extraction, manufacturing, disposal of the raw and auxiliary materials (VDI) and use of product.

drainage basin: Area from which direct surface run-off from precipitations drains by gravity into a stream or other water body (based on discussions on draft ISO 14046).

elementary flow: Material or energy entering the system being studied that has been withdrawn from the environment without previous human transformation, or material or energy leaving the system being studied that is released into the environment without subsequent human transformation (source: ISO 14040:2006 and 14044:2006).

functional unit: Quantified performance of a product system for use as a reference unit (ISO 14040:2006 and 14044:2006).

GHG Product Protocol: refers to the *GHG Protocol: Product Life Cycle Accounting and Reporting Standard.*

GHG Protocol scope 3: refers to the *GHG Protocol: Corporate Value Chain (Scope 3) Accounting and Reporting Standard.*

intermediate flow: Product, material or energy flow occurring between unit processes of the product system being studied (ISO 14040:2006 and 14044:2006).

life cycle assessment (LCA): Compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its life cycle.

non-comparative chemical product footprint study: Chemical product footprint study of one or more chemical products without any comparative assertion.

non-renewable energy consumption: Non-renewable sources of energy include fossil and nuclear energy; non-renewable energy consumption represents difference between CED and renewable energy consumption.

primary data: Data from specific operations in the studied product's life cycle that is measured (GHG Product Protocol)

reference flow: Amount of product on which the results of the study are based (GHG Product Protocol).

renewable energy consumption: Renewable sources of energy include wind power (both onshore and offshore), solar power (thermal and photovoltaic), hydroelectric power, tidal power, geothermal energy and biomass (including biofuels, bioliquids and waste from biomass); peat and biomass from primary forests are considered non-renewable (*ILCD Handbook*).

secondary data: Process data that is not from specific processes in the studied product's life cycle (GHG Product Protocol).

water withdrawal: Anthropogenic removal of water from any water body or from any drainage basin, either permanently or temporarily (based on discussions on draft ISO 14046).

3. Report template for chemical product footprint

The following template is to be used to report chemical product environmental footprint according to the present guidance.

Color code:

🟦 Requirements of ISO 14040:2006 and 14044:2006 standards

🟥 Mandatory *Life Cycle Metrics for Chemical Products* guidance requirements (“shall” requirements)

🟧 *Life Cycle Metrics for Chemical Products* guidance requirements implying justification if not applied (“should” requirements)

» Additional elements from the reporting template

» Title of the study.

» Commissioner and performer of the study.

» Date of the report.

🟦 Statement that the study has been conducted according to the requirements of the *Life Cycle Metrics for Chemical Products* guidance and according to the ISO 14040:2006 and 14044:2006 standards.

🟥 Explain and document deviation from the ISO 14040:2006, if any.

» Specifications/contact list to access the detailed methodological report.

1. Scope

1.1. Goal and scope definition

1.1.1. Intended application(s) of the study

🟥 State the intended application(s) of the chemical product footprint results in a precise and unambiguous way.

1.1.2. Reasons for carrying out the study

🟥 Explain the reasons for carrying out the chemical product footprint study, name the drivers and motivations, and especially identify the decision context. State clearly the business goal of the study.

🟥 State clearly the business goal.

1.1.3. Target audience

🟥 State the target audience of the study, i.e., to whom the results of the study are intended to be communicated.

1.2. System boundaries

1.2.1. System boundaries description

🟥 State if the system boundaries are “cradle-to-grave” or “cradle-to-gate”.

🟦 Describe all life cycle stages included.

🟥 Quantify energy and material inputs and outputs and assumptions about electricity production.

1.2.2. Limitation statement

🟥 If the system boundaries are “cradle-to-gate”, justify this choice and detail limitations for the use of the study.

🟥 Justify any specific additional stage exclusions.

1.3. Functional unit

1.3.1. Function description

🟦 State all relevant product(s) performance characteristics and relation to the functional unit.

1.3.2. Functional unit description

🟥 Provide the functional unit, defined consistently with the goal and scope of the study, and the result of its performance measurement.

1.3.3. Comparability statement (only for a comparative study)

🟧 Provide the results of the comparability assessment of the compared products according to the following elements:

- Equal benefit provided to the customer (detail chosen quality criteria);
- Functionality related to the main function of the solution;
- Technical quality, such as stability, durability and ease of maintenance;
- Additional functions rendered during use and disposal.

🟦 Describe the equivalence of the systems being compared in accordance with ISO 14044:2006 section 4.2.3.7.

1.3.4. Duration of the functional unit

🟥 For cradle-to-grave studies, report the time over which the function is provided; explain how this duration has been determined in relation to the product lifetime.

2. Methodological choices

2.1. Choices for impact categories and flows

🟥 List all impacts, energy indicators and flows chosen for the study and associated assessment methods. Justify deviations from the *Life Cycle Metrics for Chemical Products* guidance recommendations (sections 4.5.1 and 4.5.2).

- 🟥 Describe or refer to all value choices used in relation to impact categories, characterisation models, characterisation factors, and elsewhere in the impact assessment results. Justify their use and their influence on the results, conclusions and recommendations.
- 🟦 If normalisation, grouping or weighting is used in the study, please refer to ISO 14044:2006 requirements and specify the assumptions made.

2.2. Allocation rules between co-products

- 🟥 Describe allocation method with regard to the *Life Cycle Metrics for Chemical Products* guidance decision tree (section 5.2.1.2.).

2.3. Attribution of recycling benefits

- 🟥 Describe methodological choices regarding attributions for recycling.
- 🟧 In cases where a consensus along the value chain has been defined, state the consensus to which the chosen attribution method refers.

- 🟧 State if the EU PEF 50/50 attribution method has been applied or justify any deviation from this method.

- 🟥 Assess discrepancy in comparison to the results using the EU PEF 50/50 methodology in a sensitivity analysis.
- 🟥 Provide the results with and without the recycling credit attribution.

2.4. Avoided emissions

- 🟥 Describe how avoided-emissions methodological choices have been applied according to the *Addressing the Avoided Emissions Challenge* guidelines, October 2013.

2.5. Bio-based carbon storage

- 🟥 State if either an internal or external review has been performed for the assessment of fossil and bio-based carbon emissions.
- 🟥 Quantify the carbon stored in the raw biomass.
- 🟥 In case of a cradle-to-gate study, describe at least qualitatively the end-of-life of the product and its impact on the carbon elementary flow balance.

2.6. Other GHG-related issues

2.6.1. Carbon storage and delayed emissions

- 🟧 Assess the sensitivity of carbon credits associated with temporary carbon storage or delayed emissions when interpreting the global warming impact results.

2.6.2. Direct land-use change/indirect land-use change

- 🟥 Describe all direct land-use change/indirect land-use change methodological choices and parameters according to the *Life Cycle Metrics for Chemical Products* guidance methodology (section 5.2.6).

3. Data sources

3.1. Life cycle inventory analysis procedures

- 🟦 Describe data collection and calculation procedures used for the life cycle inventory analysis.

3.2. Data source description

- 🟥 Specify main data source per unit process, with the category and origin of data, as follows:
  - Data category (primary or secondary data)
  - Origin of data (for primary data only)
  - Data source type (for secondary data only):
    - Inventory data sets from recognised sources
    - Industry average eco-profiles published by associations or federations
    - Results of LCA studies published in the literature
    - Generic databases
    - Proxy data
    - Technical literature.

3.3. Data used

- 🟦 Describe the main values, data and assumptions used in the study.

4. Results and interpretation

- 🟦 List the chemical environmental footprint study results.
- 🟦 List all limitations of the results relative to the defined goal and scope of the study.
- 🟦 Detail the relationship of the impact assessment results to the inventory results.

5. Quality assessment

5.1. Quality management

5.1.1. Data quality indicators

- 🟥 Assess the data quality scoring assessment at the life cycle stage level for each unit process with a significant contribution (>10 percent) to at least one environmental impact according to the data quality indicators. Provide aggregated results.

5.1.2. Cut-off

- 🟥 Describe cut-off criteria and assumptions, effect of selection on results, and detail mass, energy and environmental cut-off criteria.
- 🟥 Detail if any elements from the following list have been found to be material and state if the element has been included in the chemical product footprint study scope:
  - Business travel (according to the GHG Protocol scope 3 definition);
  - Employee commuting (according to the GHG Protocol scope 3 definition);
  - Investments (according to the GHG Protocol scope 3 definition);
  - Infrastructure life cycle impacts;

- Energy consumption and goods not directly related to the product’s production, for example: recreation facilities, canteen, administration and R&D related activities.

🟥 In case it is not feasible to apply these exclusions (in particular if data sets do not allow it), detail these exclusions in a specific statement.

5.1.3. Data management plan

🟧 Include a statement for the user to check periodically if the chemical product footprint is valid over time and specify where necessary updated information will be available.

🟥 State any deviation from the GHG Product Protocol Data Management Plan Checklist (see Appendix 9) in the data management of the chemical product environmental footprint analysis.

5.2. Uncertainties

5.2.1. Qualitative description of uncertainties

🟥 Describe uncertainties qualitatively for each life stage.

5.2.2. Quantitative uncertainty assessments (optional)

» Quantify the uncertainties quantitatively for each life stage (optional).

5.3. Sensitivity analysis

🟦 Provide the results of sensitivity analysis assessing the robustness of the conclusions with regard to data choices, assumptions and methodological choices.

5.4. Critical/peer review

🟥 State the nature of the review performed and the name and affiliation of critical or peer reviewer(s), and provide main conclusions of the review and responses to recommendations. When the comparative assertion is intended to be disclosed to the public:

- Describe the critical review process;
- State whether or not international acceptance exists for the selected category indicators and justifications for their use;
- Assess the scientific and technical validity and environmental relevance of the category indicators used in the study.

6. Conclusion

🟦 Describe conclusions and recommendations of the study consistent with the study goal.

7. References

» List all external references used for the report.

4. Decision tree on the impact categories to communicate

The level of requirements regarding impact categories described in section 4.5.1 have been agreed on by the authors of this guideline based on following decision tree.

Decision tree on the impact categories to communicate and recommended assessment methods

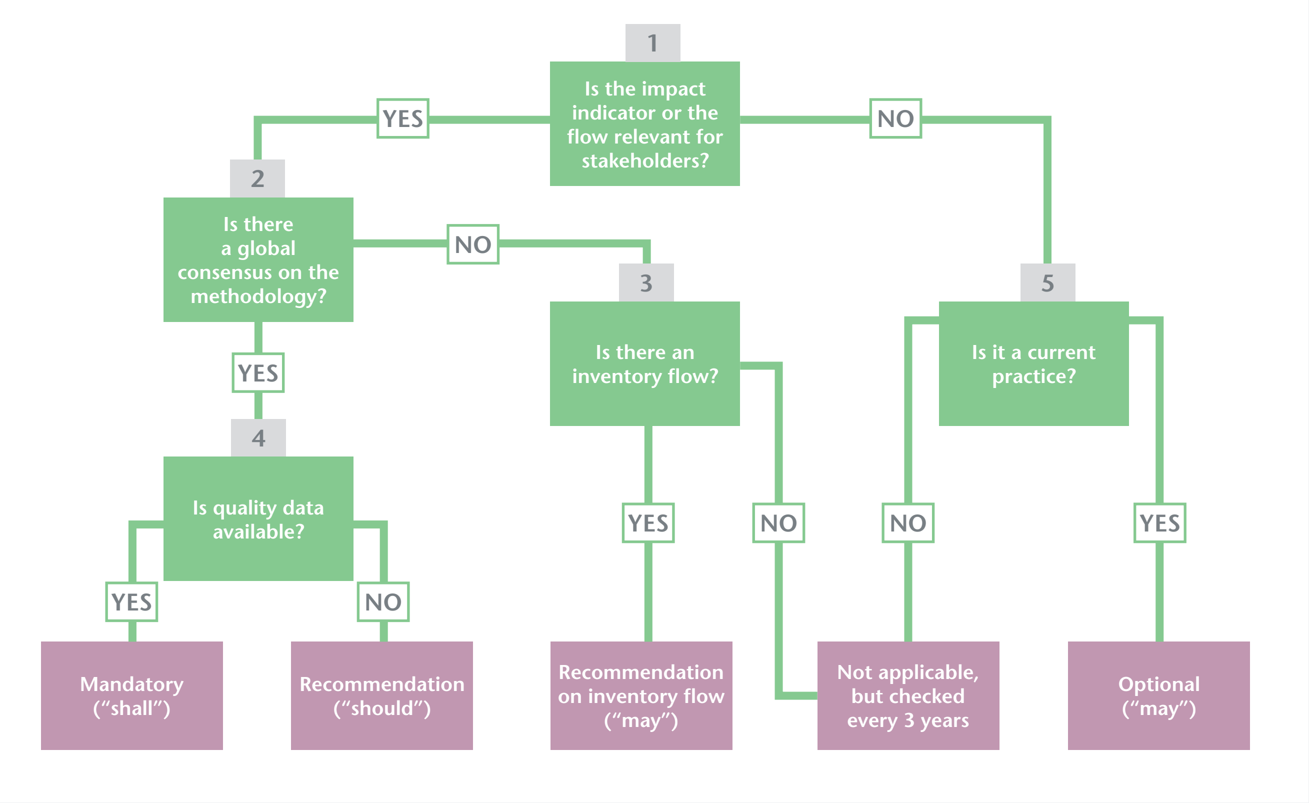


Figure 1: Decision tree on the impact categories to communicate and recommended assessment methods

All requirements and recommendations of impact categories to be communicated are based on: i) inquiries involving companies from the working group (AkzoNobel, BASF, DSM, Eastman, Evonik, Henkel, Mitsubishi Chemical Holdings, SABIC, SCG chemicals, Solvay); and ii) a survey involving a panel of stakeholders including academics, governmental bodies, non-governmental organisations (NGOs), suppliers and clients engaged in the process.

Decisions on the recommended impact assessment methods to be used for communication have been made based on a consensus between the working group companies and following the decision tree.

For instance, the impact of human toxicity potential is relevant for many stakeholders (question 1), but there is no global consensus on a reliable methodology (question 2), though inventory flows do exist (question 3). Therefore, the guidance requires users to include the human toxicity category in the communication ("shall"), but the use of the USEtox recommended assessment method is optional ("may").

In addition, on a case-by-case basis, some trade-off may be necessary. Some impacts may be regarded as not relevant for certain stakeholders, but the company may consider them relevant for the chemical sector or other stakeholders. In that case, communication on those impacts is optional ("may").

5. Secondary data sources

Models and sources listed in this section are the best currently available and may need to be revised as newer resources become available. The list is not exhaustive, and is expected to change over time.

A. Life cycle inventory (LCI) data sets

a) Industry average eco-profiles published by industry associations

The following table summarises the main information provided by LCI data sets.

Industry	Website	LCI data sets included
PlasticsEurope: Association of plastics manufacturers	http://www.plasticseurope.org/plasticssustainability/eco-profiles.aspx	Main plastics monomer and polymer families: Basic precursors, polyolefin (PO), PVC, PET, acrylic, styrenic, polyamide (PA), epoxy, polycarbonate (PC), polyurethane (PU) and other polymers, monomers & reactive precursors
FEFCO: European Federation of Corrugated Board Manufacturers & CCB - Cepi ContainerBoard	http://www.fefco.org/technical-documents/lca-database	Corrugated base papers from primary fibres: kraftliner, white top kraftliner and semichemical fluting Corrugated base papers from recovered papers: testliner, white top testliner and wellenstoff Corrugated board sheets and boxes
World Steel Association	http://www.worldsteel.org/contact-us/lca-lciForm.html	15 main finished products of the steel industry: hot rolled coil (with and without pickling), cold rolled coil (with and without finishing), hot dip and electrically galvanized sheet, painted sheet, tinplate and tin-free sheet, welded and UO pipe
EAA: European Aluminium Association	http://www.alueurope.eu/sustainability/life-cycle-assessment/	4 types of data set: - Primary aluminium production, one "produced in Europe" and one "used in Europe" (with imports) - Semi-finished aluminium production: sheet, profile and foil and extrusion - Clean process scrap remelting - Recycling of end-of-life aluminium products
Glass Fibre Europe	http://www.glassfibreeurope.eu/sustainability/life-cycle-assessment/	No LCI data set 2012 *Life cycle assessment of CFGF - Continuous Filament Glass Fibre Products* report: - Dry chopped strands - Wet chopped strands (7 to 14 percent of humidity) - Direct rovings (dry products) - Assembled rovings (dry products)
European Coil Coating Association	http://www.prepaintedmetal.eu/I_have_a_passion_for/the_environment/LCI	See the World Steel Association website to get LCI
	http://www.worldsteel.org/steel-by-topic/life-cycle-assessment.html	LCI upon request on World Steel Association website
Inventory Database for Environmental Analysis (IDEA)	http://www.milca-milca.net/download-files/MiLCAguidebook_En.pdf	LCI data sets are available in gate-to-gate type, including agriculture and fisheries, mining, construction and civil construction and other non-manufacturing, food and beverages, textiles, chemicals, ceramics and building materials, metals, machinery, and other manufacturing, electricity, gas, water and sanitation, etc. The classification for IDEA is prepared based upon classification by industry and commodity. By coding and managing all products with this IDEA classification, it is expected to provide an exhaustive data set conveniently. The total number of data sets is more than 3,000.

Supporting information	LCI available as
Methodology report common to all LCI data sets	Complete and aggregated LCI data set in Excel datasheet format - free download
2012 Report on the European Database for Corrugated Board Life Cycle Studies	Disaggregated information for each paper category in the report: raw material, additives, packaging material, transportation, energy and water inputs, emissions to air and water and residues - free download
Methodology package: product descriptions, methodology report and recycling methodology	Complete and aggregated LCI data set in Excel datasheet format - upon request
2013 methodology report: *Environmental Profile Report for the European Aluminium Industry*	Disaggregated information for each aluminium category in the report: raw material, additives, energy and water inputs, emissions to air and water and wastes - free download
2012 methodology report and peer review report Complementary qualitative information on CFGF	Impact assessment results for the CFGF products LCA of CFGF products report from PwC Free download Further information upon request
NA	NA
2012 sustainability report	Free download by email
IDEA is the standard equipment inventory database for MiLCA LCA software. IDEA has been jointly developed since FY 2008 by the National Institute of Advanced Industrial Science and Technology (AIST) and Japan Environmental Management Association for Industry (JEMAI).	In MiLCA software

b) *Generic databases*

Public databases

The European reference Life-Cycle Database (ELCD) is recognised at the European level. Data sets are available for free download on the dedicated Joint Research Centre (JRC) website. All data sets are reviewed, and detailed qualitative information is provided alongside quantitative LCI (in particular regarding the quality of the data set).

Industry	Website	LCI data sets included	Supporting information	LCI available as	Important methodological assumptions
European reference Life Cycle Database (ELCD)	http://lca.jrc.ec.europa.eu/lcainfohub/datasetArea.vm	LCI data set from front-running EU-level business associations and other sources for key materials, energy carriers, transport, and waste management	Complete detailed information for each data set: process information, modelling and validation, administrative information, LCA report and review report	xml files - free download	Detailed for each data set
National Renewable Energy Laboratory (NREL)	http://www.nrel.gov/lci/	Includes 633 processes detailed as follows: air transportation (1), chemical manufacturing (84), crop production (34), electrical equipment, appliance, and computer manufacturing (2), fabricated metal product manufacturing (1), forestry and logging (80), mining (except oil and gas) (6), non-metallic mineral product manufacturing (4), oil and gas extraction (3), paper manufacturing (2), petroleum and coal products manufacturing (2), plastics product manufacturing (3), plastics and rubber products manufacturing (1), primary metal manufacturing (23), rail transportation (1), transit and ground passenger trans. (46), transportation equipment manufacturing (5), truck transportation (102), utilities (125), waste management and remediation service (22), water transportation (6), wood product manufacturing (59), biomass (21)	Global generic report and information fields in data sets (not compliant with ELCD)	SPOLD and Excel	Detailed for each data set
Life Cycle Assessment Society of Japan (JCLA) database	http://lca-forum.org/database/	LCI data sets are available for product manufacturing, disposal and recycling processes that were voluntarily collected by 54 industrial associations and covering the following sectors: energy, materials, machinery, electronic/electric, IT, buildings and others	JLCA database was developed by Life Cycle Assessment Society of Japan.	Free for JLCA members	Detailed for each data set
Inventory Database for Environmental Analysis (IDEA)	http://www.milca-milca.net/download-files/MiLCAguidebook_En.pdf	LCI data sets are available in gate-to-gate type, including agriculture and fisheries, mining, construction and civil construction and other non-manufacturing, food and beverages, textiles, chemicals, ceramics and building materials, metals, machinery, and other manufacturing, electricity gas, water and sanitation, etc. The classification for IDEA is prepared based upon classification by industry and commodity. By coding and managing all products with this IDEA classification, it is expected to provide an exhaustive data set conveniently. The total number of data sets is more than 3,000.	LCI data sets and LCA tool	IDEA is the standard equipment inventory database for MiLCA LCA software. IDEA has been jointly developed since 2008 by the National Institute of Advanced Industrial Science and Technology (AIST) and Japan Environmental Management Association for Industry (JEMAI).	In MiLCA software

Other databases (available for purchase)

Industry	Website	LCI data sets included	Supporting information	LCI available as
ecoinvent – the Swiss Centre for Life Cycle Inventories	http://www.ecoinvent.org/database/	LCI data sets in the areas of agriculture, energy supply, transport, biofuels and biomaterials, bulk and specialty chemicals, construction materials, packaging materials, basic and precious metals, metals processing, ICT and electronics, as well as waste treatment	Methodological reports by processes categories	SPOLD files-purchase prices on the website
GaBi	http://www.gabi-software.com/databases	More than 5,000 life cycle inventory data sets based on primary data collection, including agriculture, building and construction, chemicals and materials, consumer goods, education, electronics and ICT, energy and utilities, food and beverage, healthcare and life sciences, industrial products, metals and mining, plastics, retail, service sector, textiles	Metadata in compliance with ILCD	SPOLD Files and Excel
DEAM	http://ecobilan.pwc.fr/fr/boite-a-outils/deam.jhtml	Transportation, energies, polymers, packaging, steel and stainless steel, aluminium; other data available or to be made upon request (case by case) in many sectors	Metadata in compliance with ILCD	SPOLD Files and Excel
JEMAI-LCA	http://www.milca-milca.net/english	Main database: JEMAI-LCA standard database: Includes more than 500 processes on iron, steel, non-ferrous metal, plastic, rubber, chemical, oil, coal, ceramics and paper Additional databases: JEMAI-LCA option data pack: Includes an additional 1,000 processes on chemical, steel, rubber and recycling (only available in Japanese)	Not available	Not available

Appendix 6 provides information on recommended data sources for energy and transport data sets.

B. Technical literature and process simulations

Industry	Website	Technical information included	Information available as
IHS Chemicals (*Chemical Process Economic Program and Chemical Economics Handbook*)	http://www.ihs.com/login-chemical.aspx	Detailed information on chemical production processes via different technologies and regions This information can be used to construct LCIs Nexant, other consultants offer similar services	Paid subscription required
Engineering design packages	-	Chemical producers develop detailed heat and material balances for chemical plants when the plants are being designed, which can also be reliable sources of inventory data	Internal use only
Aspen Plus	http://www.aspentech.com/products/aspen-plus.aspx	Computer simulation tools, such as Aspen Plus, are used to apply chemical engineering principles to design conceptual chemical plants for the development of LCI data	Paid subscription required
Ullmann's Encyclopedia of Industrial Chemistry	http://onlinelibrary.wiley.com/doi/10.1002/14356007.a10_045.pub3/abstract	Chemical process and facilities information; properties of chemical substances Subject areas include notably: inorganic and organic chemicals, advanced materials, pharmaceuticals, polymers and plastics, metals and alloys, biotechnology and biotechnological products, food chemistry, process engineering and unit operations, analytical methods and environmental protection	Paid book or PDF file
Kirk-Othmer Encyclopedia of Chemical Technology	http://scd.univ-tlse3.fr/kirk-othmer-encyclopedia-chemical-technology	Chemical process and facilities information; properties of chemical substances; latest research review including environment and health	Paid book or PDF file

6. Examples of data sources for generic data

The following tables present the main existing data sources for the most frequently used generic data (for energy production and combustion, electricity production and transport use), as well as the results of a survey performed among working group companies.

This list is provided as a guide to common existing data sources currently available. It is not exhaustive, and it is expected to change over time.

Energy production data

	Ecoinvent	ELCD	NREL	DEAM	GABI	Other	Focus on most used data	User's Comments
Heavy fuel oil	2005 general multi-output refinery operations	2003	Crude oil at refinery 2010	ETH 96	2009 with mix by region		Heavy fuel oil, at refinery / RER U; based on ecoinvent v2.2	Energy production is rarely used, since our inventories mainly concern energy consumption on our sites. We use the data sets which both include production, distribution and combustion of energy sources.
Panel data	3	-	-	-	1	-		-
Light fuel oil	2005 general multi-output refinery operations	2003	Crude oil at refinery 2010	ETH 96	2009 with mix by region		Light fuel oil, at refinery / RER U; based on ecoinvent v2.2	
Panel data	3	-	-	-	1	-		-
Gasoline		2003	Crude oil at refinery 2010	ETH 96	2009 with mix by region		Petrol, low sulphur, at refinery / RER U; based on ecoinvent v2.2	
Panel data	2	-	-	-	1	-		-
Natural gas	1989-2005 depending on region and quality	2002	2011	PlasticsEurope 2005	2009 with mix by region	PlasticsEurope 2005	Natural gas, high pressure, at consumer / RER U; based on ecoinvent v2.2	
Panel data	2	-	-	-	2	-		-
Coal	1999-2002	2002		ETH 96	2009 with mix by region		Hard coal mix, at regional storage, UCTE U; based on ecoinvent v2.2	
Panel data	2	1	-	-	1	-		-
Lignite	83-94	2002	2003-2011	ETH 96				Not used frequently
Panel data	1	-	-	-	1	-		-
Diesel oil	2005 general multi-output refinery operations	2003	Crude oil at refinery 2010	ETH 96	2009 with mix by region		Diesel, low sulphur, at refinery / RER U; based on ecoinvent v2.2	
Panel data	1	-	-	-	1	-		-

Crude oil	2005 general multi-output refinery operations		2003-2011		2009 with mix by region		Location wise datasets for crude oil production; based on ecoinvent v2.2	
Panel data	1	-	-	-	1	-		-

Energy consumption data

	Ecoinvent	ELCD	NREL	DEAM	GABI	Other	Focus on most used data	Comment
Heavy fuel oil	1991-2000	2003	NA	ETH 96	2009 with mix by region		Heavy fuel oil, burned in industrial furnace, 1 MW, non-modulating / RER U; based on ecoinvent v2.2	
Panel data	3	-	-	-	1	-		-
Light fuel oil	1991-2000	2006	NA	ETH 96	2009 with mix by region		Light fuel oil, burned in industrial furnace, 1 MW, non-modulating / RER U; based on ecoinvent v2.2	
Panel data	4	-	-	-	1	-		-
Gasoline		2003	NA	ETH 96	2009 with mix by region			
Panel data	1	-	-	-	1	-		-
Natural gas	2000	2006	NA	ETH 96	2009 with mix by region		Natural gas, burned in boiler, atmospheric, low NOx, non-modulating / RER U; based on ecoinvent v2.2	
Panel data	4	-	-	-	1	-		-
Coal	1988-1992	NA	NA	ETH 96	2009 with mix by region		Hard coal, burned in industrial furnace, 1-10 MW / RER U; based on ecoinvent v2.2	
Panel data	4	-	-	-	1	-		-
Lignite		2002	NA	ETH 96	2009 with mix by region			Not used frequently
Panel data	1	-	-	-	1	-		-
Diesel oil	1996-2001	2003	NA	ETH 96	2009 with mix by region			Not used frequently
Panel data	1	-	-	-	1	-		-
Total	18	-	-	-	7	-		-
Panel data	1	-	-	-	1	-		-

Electricity production data

Electricity production data	Ecoinvent V3	ELCD	NREL	DEAM	GABI	Focus on most used data	User's Comments	Comment
Electricity mix						IEA	Local electricity grid mixes are mostly used. Grid mixed are based on location of production sites. But for product use, RER or UCTE or relevant grid mixes are used. Grid composition based on sales record in various regional markets is not being practised here.	
Panel data	2	-	-	-	1	1	-	-
Electricity in France						Electricity, medium voltage, production FR, at grid/FR U		
Panel data	3	1	-	-	1	-	-	-
Electricity by country in Europe	2010 recalculation	2002	NA		2008-2012	Electricity, medium voltage, production RER, at grid/RER U		
Panel data	2	-	-	-	1	-	-	-
Electricity by country in USA			2000					
Panel data	4	-	-	-	1	-	-	-
Electricity from coal	93-2000 or 2008 depending on countries (FR=93-2000)	NA	NA	CO_2, CH_4, N_{20} updated according to 2006 *IPCC Guidelines for National Greenhouse Gas Inventories;* other emission factors: *EMEP/EEA emission inventory guidebook* 2009, updated June 2010, Energy Industries, Combustion in energy and transformation industries tier 1 factors	2008-2012	"Electricity, medium voltage, at grid/US U	Hard coal, burned in industrial furnace, 1-10 MW / RER U; based on ecoinvent v2.2	
Panel data	4	-	-	-	1	-	-	Not used frequently
Electricity from nuclear		NA	NA	Bibliographic data 2011	2008-2012		From the closest country for the considered region	-
Panel data	4	-	-	-	1	-	-	Not used frequently
Electricity from hydro	2008	2002	NA	2011, source : Syndicat des Energies Renouvelables + ETH 96	2008-2012		From the closest country for the considered region	-
Panel data	4	-	-	-	1	-	-	-
Electricity from oil		NA	NA	CO_2, CH_4, N_{20} updated according to 2006 *IPCC Guidelines for National Greenhouse Gas Inventories;* other emission factors: *EMEP/EEA emission inventory guidebook* 2009, updated June 2010, Energy Industries, Combustion in energy and transformation industries tier 1 factors	2008-2012		From the closest country for the considered region	-
Panel data	4	-	-	-	1	-	-	-
Electricity from natural gas		NA	NA	CO_2, CH_4, N_{20} updated according to 2006 *IPCC Guidelines for National Greenhouse Gas Inventories;* other emission factors: *EMEP/EEA emission inventory guidebook* 2009, updated June 2010, Energy Industries, Combustion in energy and transformation industries tier 1 factors	2008-2012		From the closest country for the considered region	

Transportation data

	Ecoinvent	ELCD	NREL	DEAM	GABI	Focus on most used data	User's Comments
Rail transport – electric	2000	2005	2006	• Proportion of electric/diesel trains: Energy Efficiency Solution for Rolling Stock, Rail Infrastructure and Train Operation. http://www.railenergy.eu/scope.aspx. In Europe, 20% of trains run on diesel, 80% on electricity • Facteurs d'émissions diesel: -*Ecological Transport Information Tool for Worldwide Transports Methodology and Data Update* IFEU Heidelberg Öko-Institut IVE / RMCON Berlin – Hannover - Heidelberg, July 31th 2011 http://www.ecotransit.org/download/ecotransit_background_report.pdf	ELCD are Gabi Data	Transport freight, rail / RER U (ecoinvent v2.2); created in 2003, latest revision - 2010	Any LCA study shall be transparent about the return trip of the (possibly) empty transportation vehicle.
Panel data	4	-	-	-	-	-	-
Road transport	2005	2005-2007	2009	Sce : EMEP/EEA emission inventory guidebook 2009, updated May 2011	ELCD are Gabi Data	Transport, lorry 16-32t, EURO5/ RER U	
Panel data	4	-	-	-	1	-	-
Plane transport – goods	2000	2005	2006	ETH 96	ELCD are Gabi Data	Transport, aircraft, freight, intercontinental/RER U for long distance	
Panel data	3	-	-	-	1	-	-
Plane transport – passengers	2000	NA	NA	ETH 96	ELCD are Gabi Data		Rarely used
Panel data	2	-	-	-	-	-	-
Rail transport – passengers	2005	NA	NA	ETH 96	ELCD are Gabi Data		Rarely used
Panel data	2	-	-	-	-	-	-
Car passenger	2012	NA	2009	ETH 96	ELCD are Gabi Data	Transport, passenger car, EURO 4 / RER U; based on Ecoinvent v2.2	Rarely used
Panel data	3	-	-	-	-	-	-

Rail transport - diesel oil	2000	2005	2003	• Proportion of electric/diesel trains: Energy Efficiency Solution for Rolling Stock, Rail Infrastructure and Train Operation. http://www.railenergy.eu/scope.aspx. In Europe, 20% of trains run on diesel, 80% on electricity • Facteurs d'émissions diesel: -*Ecological Transport Information Tool for Worldwide Transports Methodology and Data Update* IFEU Heidelberg Öko-Institut IVE / RMCON Berlin – Hannover - Heidelberg, July 31th 2011 http://www.ecotransit.org/download/ecotransit_background_report.pdf	ELCD are Gabi Data	Transport freight, rail / RER U (ecoinvent v2.2); created in 2003, latest revision - 2010 or Transport, freight, rail/RER U or by country when specified	
Panel data	4	-	-	-	1	-	-
Transport barge	1998	2005	2001-2006	ETH 96	ELCD are Gabi Data	Transport, transoceanic tanker or freight / OCE U; based on ecoinvent v2.2 or Transport, barge/RER U	
Panel data	4	-	-	-	1	-	-
Transport container	2011	2005	2001-2006	ETH 96	ELCD are Gabi Data	Transport, transoceanic freight ship/OCE U	Not used frequently
Panel data	2	-	-	-	1	-	-

7. Examples of allocation for co-products

Example – Biodiesel production

Authors: Guido Vornholt (Evonik), Jean François Viot (Solvay)

Process description

The last step of biodiesel production is the transesterification of vegetable oils (e.g., rapeseed) or animal fats into the main product, the biofuel, and the co-product glycerol (also known as glycerine).

Allocation decision hierarchy

1) **Is it possible to subdivide the process into several and distinct processes to avoid allocation?**

   No, as a single reaction (transesterification) is delivering two products.

2) **Is the system delivering co-product(s) that can be replaced by easily identifiable conventional product(s)?**

   No, the glycerol available on the market is produced through various routes where glycerol is also always a co-product (e.g., soap production and fatty acid/alcohol production from various vegetable and animal feedstocks or synthetic glycerol production from propylene).

   Decision = Allocation is required

3) **Use the allocation based on the parameter describing the best underlying relations between the co-products as the main scenario.**

   The parameter that is the most representative of the relations between the biodiesel and the co-product (glycerol) is the net calorific value (NCV) energy parameter. Indeed, the main product used is a fuel; therefore, energy appears as the most relevant parameter for allocation and will be used as the main allocation method to present the conclusions.

   In addition, this allocation method follows the recommendation of the European Commission's Renewable Energy Directive 2009/28/CE: *"Co-products from the production and use of fuels should be taken into account in the calculation of greenhouse gas emissions. The substitution method is appropriate for the purposes of policy analysis, but not for the regulation of individual economic operators and individual consignments of transport fuels. In those cases, the energy allocation method is the most appropriate method, as it is easy to apply, is predictable over time, minimises counter-productive incentives and produces results that are generally comparable with those produced by the substitution method. For the purposes of policy analysis, the Commission should also, in its reporting, present results using the substitution method."*

4) **If market prices of the several co-products are available, do they differ by more than 20% (average market price over 3 years)?**

   Yes, between 2010 and 2013, the average biodiesel price was 1.3 €/kg (variation between 1 and 1.6 €/kg), whereas for glycerol the average price was 0.3 €/kg (variation between 0.25 and 0.35 €/kg). The average price of biodiesel is more than four times higher than the average price for glycerol.

5) **Perform at least two allocation methods as a sensitivity analysis: economic allocation and another allocation based on another parameter (not correlated to the previous two), such as mass, energy or stoichiometry, and present the results according to these methods in the conclusions of the study.**

   Economic and mass allocation can be studied as sensitivity analysis.

Results (with illustrative values for allocation method parameters)

Allocation method	Biodiesel	Glycerol	Environmental impact of biodiesel	Environmental impact of glycerol
Energy (NCV)	37,000 MJ/t	17,000 MJ/t	98%	2%
Mass	1 t	0.05 t	95%	5%
Economic (sales price)	1,480 €/t	300 €/t	99%	1%

Table 1: Results (with illustrative values for allocation method parameters)

Conclusion

In this example, allocation methods do not have an important influence on the distribution of the environmental impacts between biodiesel and glycerol (all methods reveal an influence of < 5 percent impact for glycerol). The main results shall be presented according to the energy allocation, and the results of the sensitivity analysis on mass and economic allocation shall be presented to complete the interpretation of the results.

Example – Ammonia process

Authors: Ananda K. Sekar, Sreepadaraj Karanam, Gretchen Govoni, Avantika Shastri (SABIC)

Process description

The industrial synthesis of ammonia is based on a high-pressure reaction between H_2 and N_2. The overall scheme of the process is outlined below:

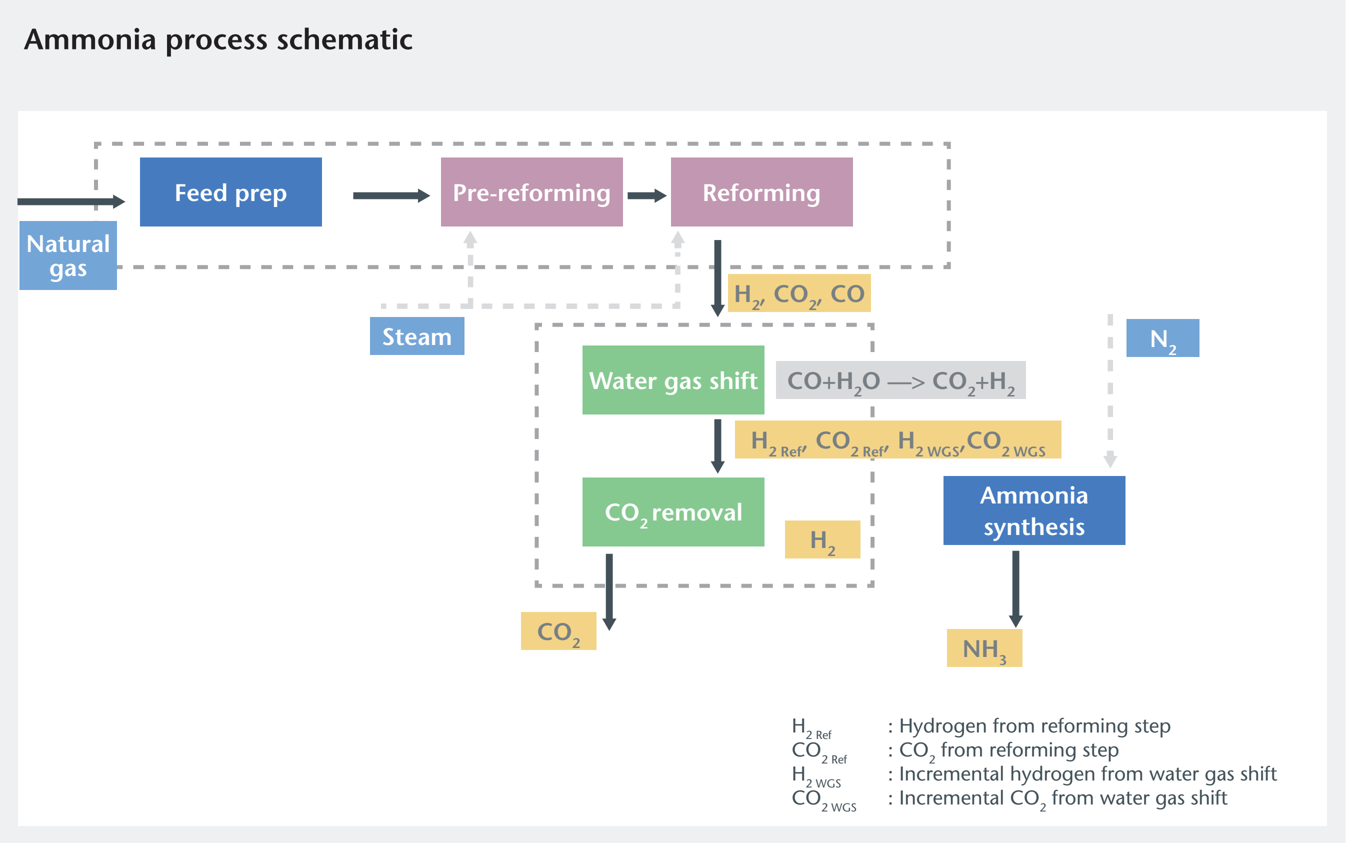
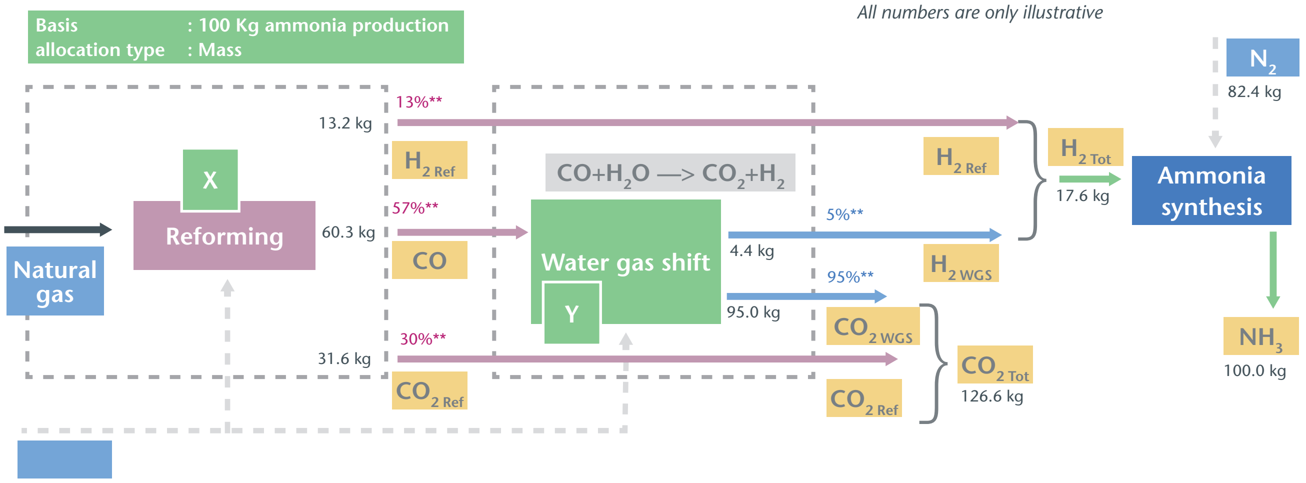


Figure 1: Ammonia process schematic

1. Feed prep: This step involves the removal of sulphur and chlorides, which may be catalyst poison or pose "metal corrosion" issues in downstream sections of the plant, from the natural gas feed.
2. Reforming: This is carried out as a single step or as two steps (pre-reforming + primary reforming). The reaction is primarily based on the reaction of natural gas with steam to primarily form hydrogen and carbon oxides. While hydrogen is a desired product from the process, carbon oxides are either unwanted by-product (for stand-alone ammonia facilities) or desired co-product for urea production (for integrated urea-ammonia complexes that use carbon dioxide and ammonia as feedstocks for urea synthesis).
3. Water gas shift: Regardless of these end objectives, "water gas shift" reactions are utilised to maximise hydrogen yield from the overall process. This involves the reaction of carbon monoxide with water to form carbon dioxide and incremental hydrogen.
4. CO_2 removal: This step is required to separate carbon dioxide from the product stream. This step also involves the separation of any residual carbon monoxide and methane. Methanation (not shown in the schematic) is another supporting process step that helps convert carbon oxides to methane, which can more easily be separated from the hydrogen product stream.
5. Ammonia synthesis: This step involves the high-pressure reaction of nitrogen with hydrogen to form ammonia. It is important to note that there is no participation of a carbon dioxide co-product in this step.

Ammonia process – mass allocation for sub-process units



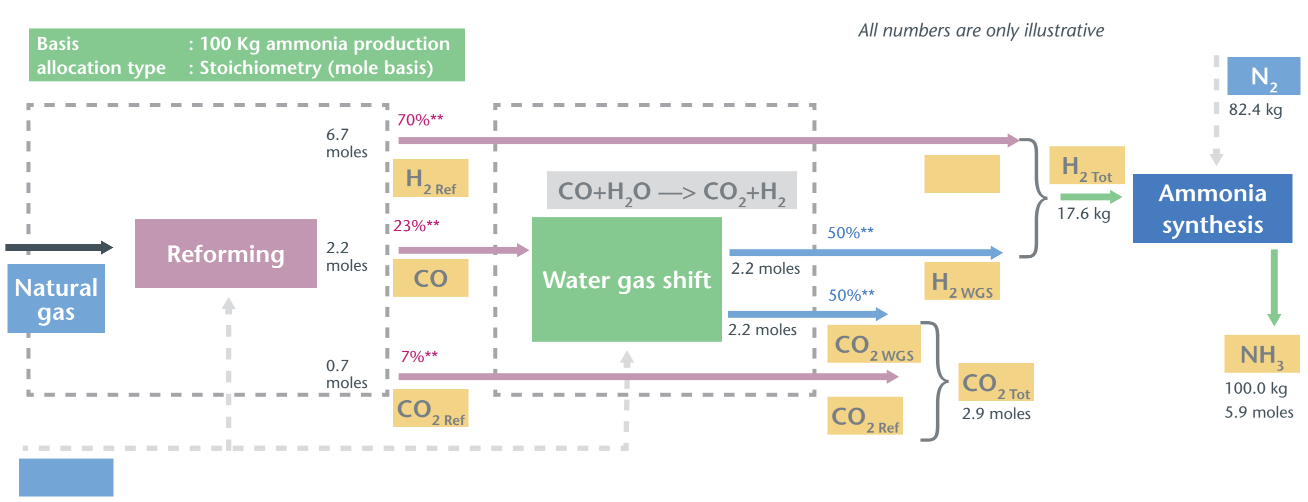
$$CO_{2\ Tot} = [0.13Y + (0.67Y + X)0.05] = 0.16Y + 0.05X$$
$$NH_{3\ Tot} = [0.13Y + (0.67Y + X)0.95] = 0.84Y + 0.95X$$

*** % allocation share based on "mass"*

H_2 Ref : Hydrogen from reforming step
CO_2 Ref : CO_2 from reforming step
$H_{2\ WGS}$: Incremental hydrogen from water gas shift
$CO_{2\ WGS}$: Incremental CO_2 from water gas shift
X : Process burdens from reforming step & upstream
Y : Process burdens from WGS step

Figure 2: Ammonia process – mass allocation for sub-process units

Ammonia process – stoichiometry-based allocation for sub-process units



$$CO_{2\ Tot} = [0.70Y + (0.23Y + X)0.50] = 0.82Y + 0.50X$$
$$NH_{3\ Tot} = [0.07Y + (0.23Y + X)0.50] = 0.18Y + 0.50X$$

*** % allocation share based on "stoichiometry"*

H_2 Ref : Hydrogen from reforming step
CO_2 Ref : CO_2 from reforming step
$H_{2\ WGS}$: Incremental hydrogen from water gas shift
$CO_{2\ WGS}$: Incremental CO_2 from water gas shift
X : Process burdens from reforming step & upstream
Y : Process burdens from WGS step

Figure 3: Ammonia process – stoichiometry-based allocation for sub-process units

Allocation decision hierarchy

1. **Is it possible to subdivide the process into several and distinct processes to avoid allocation?**

   As described in the previous section, ammonia synthesis is a multi-step process. With the exception of the ammonia synthesis step, all of the other reaction steps are attributable to both carbon dioxide and hydrogen. Steam methane reforming typically produces around 3:1 syngas (mole ratios of H_2:CO). In the shift reaction, every mole of carbon monoxide converts to 1 mole of hydrogen and 1 mole of CO_2. The overall reaction produces around 1.3 kg CO_2 per kg ammonia.

   As shown in figures 2 and 3 above, if "mass allocation" were applied for individual process steps, then burdens per kg of hydrogen (hence per kg ammonia) would be less than that per kg of carbon dioxide. This is partly due to the fact that hydrogen carries lesser burdens due to its lighter weight; also, the majority of hydrogen production is via the reforming step, while the majority of the carbon dioxide production is via the water-gas shift (WGS) step, which will also carry burdens of carbon monoxide from the reforming step apart from burdens for the WGS step.

   In contrast, if stoichiometry (mole)-based allocation is applied for individual process steps, then burdens per kg of hydrogen will be substantially higher than that per kg of carbon dioxide. These are also better explained by the equations below each figure.

   However, it is very difficult to argue for stoichiometry or mass to be the right allocation basis since they are only different units of measurement.

   Note: All the above allocation scenarios only apply for the reforming and WGS steps. For the ammonia synthesis step, all burdens will be attributable to the ammonia product alone (since there are no co-products from this particular step).

2. **Is the system delivering products/services that can replace an easily identifiable conventional product/service (e.g., grid electricity)?**

   No.

3. **Is it possible to expand the system to other similar processes (only in the case of very specific and identifiable products/services)?**

   In this process, system expansion cannot be applied to the carbon dioxide co-product since there is no other commercially dominant route for CO_2 production. CO_2 production is mostly tied to reforming. While some processes are interested in maximising carbon monoxide as a desired co-product along with hydrogen (herein carbon dioxide is an undesired co-product), other reforming processes that are linked to ammonia synthesis produce carbon dioxide as a desired co-product that could be diverted to urea production.

   Decision = Allocation is required

4. **If market prices of the several co-products are available, do they differ by more than 20% (average market price over three years)?**

   Yes. Although carbon dioxide has some marketability as a product (carbonation of beverages, wastewater pH adjustment, etc.), it is relatively smaller by volume compared to the ammonia market. It also does not have an established global supply chain and market. In addition, carbon dioxide may also be associated with abatement or externality costs depending on the existence of regulations and/or carbon markets. In the context of ammonia-urea integrated complexes, a portion of ammonia is sold as a product to external markets and the rest is diverted to urea production. In such cases, associating market value to ammonia and carbon dioxide (both ammonia and carbon dioxide are necessary feedstocks for the urea process) may be complicated.

Allocation could be based on two options:
1. Mass, all burdens to ammonia;
2. Mass, all products.

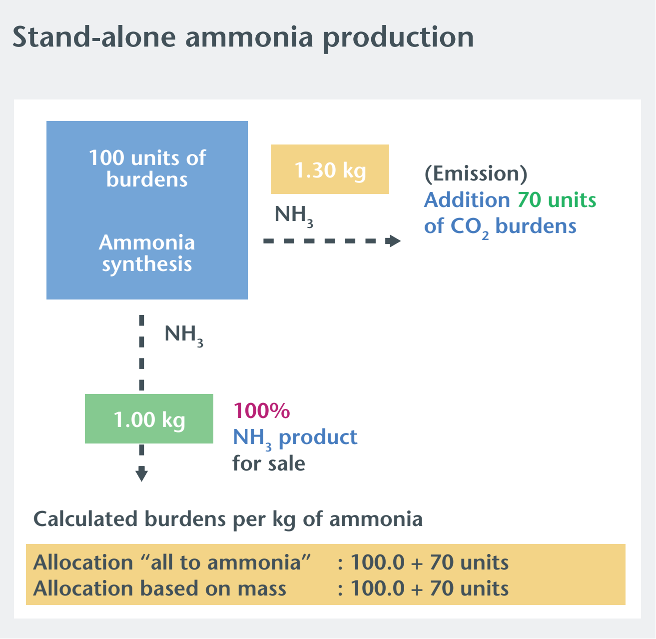


Figure 4: Stand-alone ammonia production

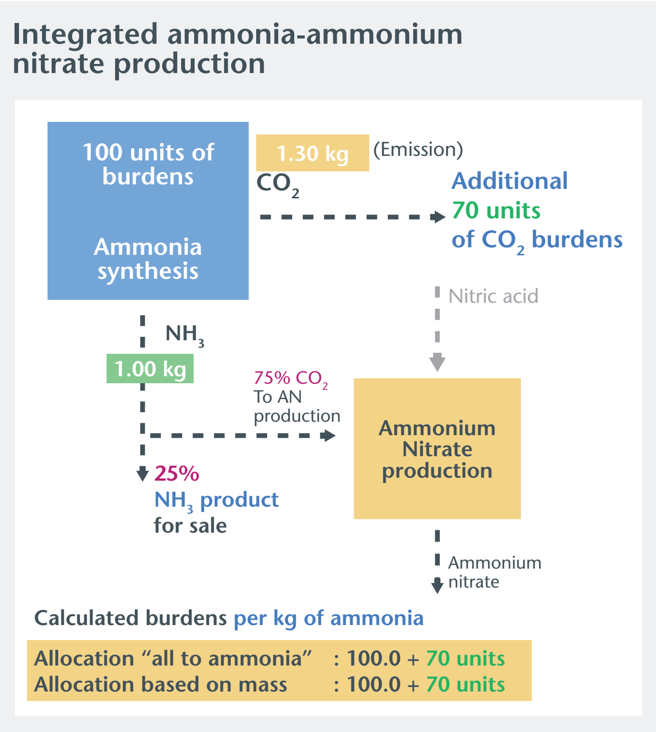


Figure 5: Integrated ammonia-ammonium nitrate production

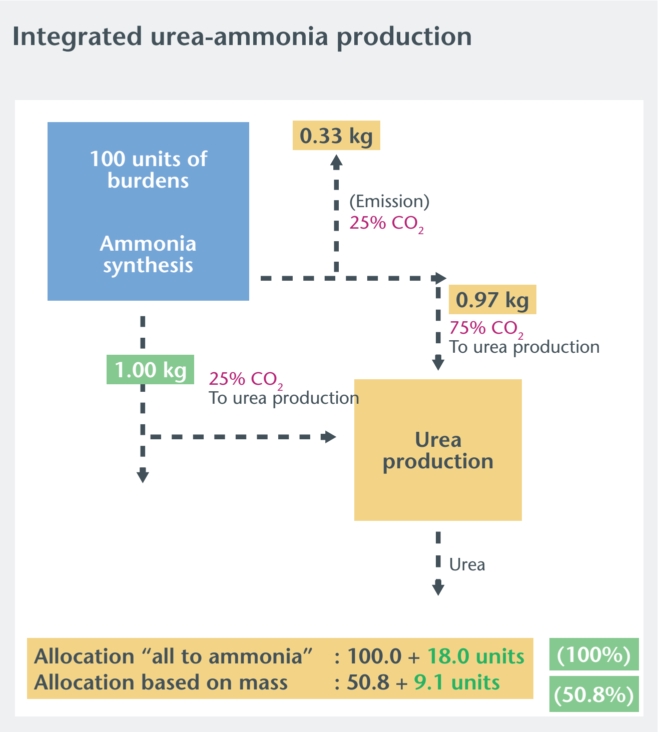


Figure 6: Integrated urea-ammonia production

The figures above are based on stoichiometry (only used here for illustrative purposes). As indicated in the figure, about 1.3 kg CO_2 is produced as a co-product for every kg of ammonia. This carbon dioxide can be used as a desired co-product (to be subsequently diverted for urea production) or as an unwanted co-product and hence treated as an emission and liability.

In the example above, a case where 25% of the ammonia produced is sold as a product and the rest (75%) will be diverted to urea production or ammonium nitrate production has been assumed. Since the urea complex consumes ammonia and carbon dioxide at nearly the same stoichiometric ratio as they are produced in an ammonia plant, 25% of the ammonia sold outside as a product will create a 25% surplus of CO_2 for the urea complex. This does not occur in cases of ammonium nitrate production wherein only ammonia is consumed in the ammonium nitrate complex (all of the carbon dioxide produced becomes an emission liability unless captured for another use).

Results

1. Mass allocation, with cut-off for CO_2

This would imply that all burdens of the process are attributable to ammonia and none to carbon dioxide. Ammonia is the key desired co-product for stand-alone plants, ammonium nitrate integrated facilities and integrated urea-ammonia complexes. But carbon dioxide is available as an additional intended co-product only for urea-ammonia integrated fertilier complexes. This provides a premise for the exploration of alternative co-product allocation scenarios for urea-ammonia integrated complexes.

However, carbon intensities reported for ammonia plants (for instance, by the International Fertilizer Association) are based on "all burdens to ammonia". In other words, "mass allocation with cut-off for CO_2". Likewise, ecoinvent data sets also use this approach for ammonia production.

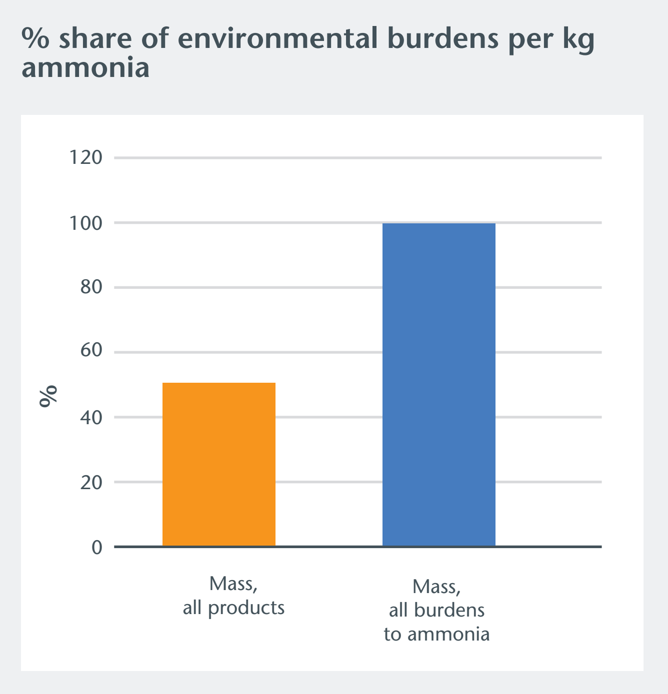


Figure 7: Share of environmental burdens for ammonia, various allocation scenarios

2. Mass, all products: This apportions equal burdens to ammonia and carbon dioxide (per kg basis).

As shown in figure 7 above, this provides an additional incentive for the recovery of carbon dioxide as a useful co-product and its utilisation for the urea process or other emerging industrial applications. This thus provides an additional incentive for all ammonia plants to explore alternatives for the capture and use of CO_2.

3. Mass, partitioned ammonia allocation

It is evident from the above discussions that for ammonia-urea integrated complexes, whenever all of the ammonia is diverted to urea production, all of the process CO_2 is consumed in urea production. Whenever a portion of the ammonia is sold externally as a product, it translates to an equivalent CO_2 liability since the urea plant can always only take ammonia and CO_2 on a proportional basis. In such a case, the ammonia diverted to the urea process can be treated as a separate product stream from the ammonia sold externally as a product. This would imply that process CO_2 burdens (emitted as a consequence of ammonia sold to the external market) should be attributable to "ammonia, sold as external product". This would imply that none of the process CO_2 emissions are attributable to "ammonia, diverted to urea production". This is illustrated in figure 8:

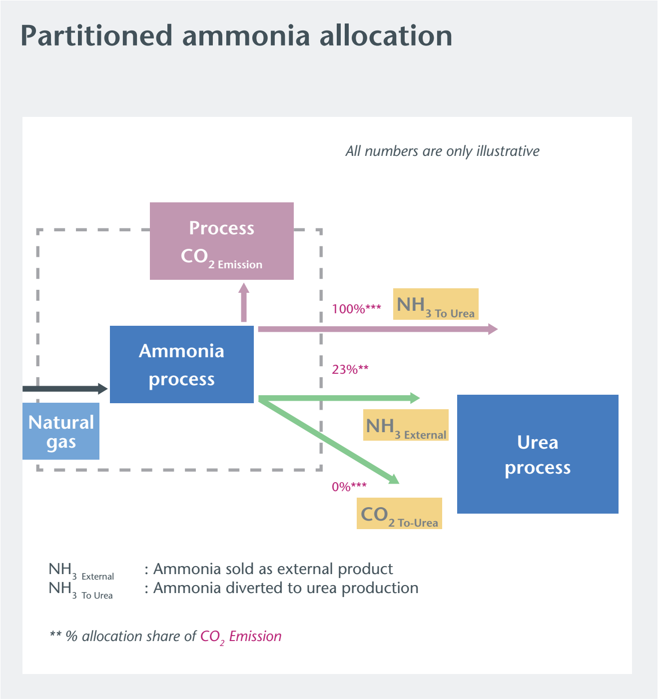


Figure 8: Partitioned ammonia allocation

Decision tree for allocation

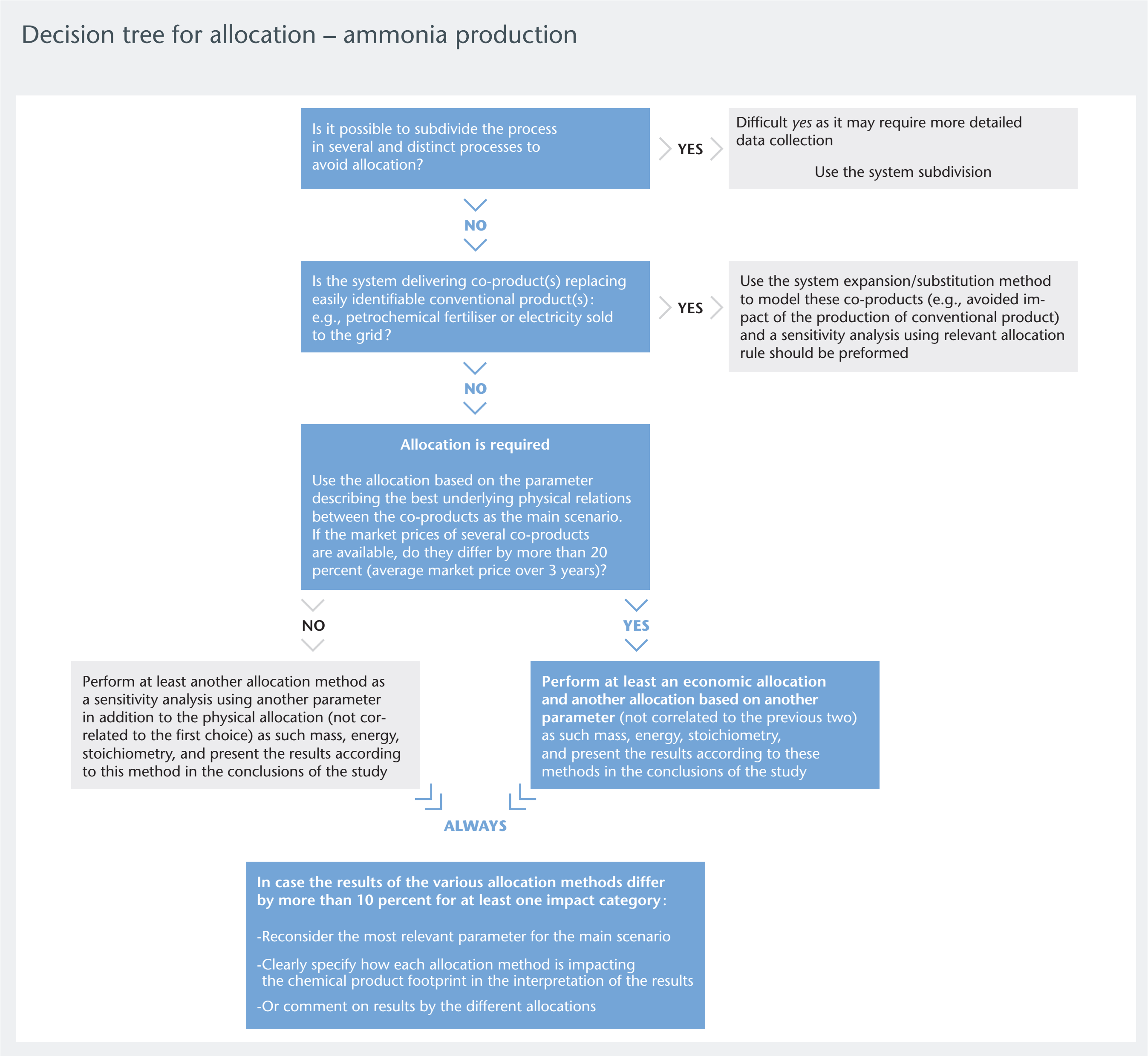


Figure 9: Decision tree for allocation – ammonia production

Conclusion

From the above discussion, it is evident that the allocation basis may significantly influence the results of the study. “Partitioned ammonia allocation” may be considered to be a fair basis of allocation of “process CO_2 burdens” between two different ammonia product streams (ammonia external vs. ammonia for urea production). THe industry may need to adopt a consistent approach for the allocation of the rest of the process burdens for LCA studies to be comparable. Since economic allocation, stoichiometry and mass allocation all have their merits and demerits, as described in figure 3, it is recommended to perform at least three other allocation approaches as part of sensitivity analysis, in order to highlight possible variations in the measured impacts based on each allocation approach being considered.

Example – Sulphuric acid production

Authors: Carmen Alvarado (AkzoNobel), Henk Bosch (DSM)

Process description

The production of sulphuric acid (H_2SO_4) is through an exothermic reaction. A fair amount of steam is produced.

Allocation decision hierarchy

1) **Is it possible to subdivide the process into several and distinct processes to avoid allocation?**
   No, as a single reaction delivers sulphuric acid and steam.

2) **Is the system delivering co-product(s) that can be replaced by easily identifiable conventional product(s)?**
   Yes, steam can otherwise be produced in a boiler burning hard coal or natural gas.

   Decision = Use system expansion/substitution

Method	H_2SO_4	Steam	Environmental impact of H_2SO_4 (GHG emissions)	Environmental impact of steam (GHG emissions)
System expansion (assuming hard coal burned in boiler)	1 t	807 MJ	-68 kCO_2eq	-79 kCO_2eq
System expansion (assuming natural gas burned in boiler)	1 t	807 MJ	-44 kCO_2eq	-55 kCO_2eq

Table 2: Results using the system expansion/substitution

The result of system expansion is negative GHG emissions for sulphuric acid. The value depends on the reference for system expansion.

Economic and mass allocation can be studied using sensitivity analysis.

3) **If market prices of the several co-products are available, do they differ by more than 20% (average market price over three years)?**
   Yes, the price of steam and sulphuric acid remains fairly constant. The difference in price among both products is higher than 20%.

Results

Method	H_2SO_4	Steam	Allocation to H_2SO_4	Allocation to steam
Mass	1 t	~ 0.3 t	77%	23%
Economic (sales price)	~100 €/t	0.005 €/MJ	96%	4%

Table 3: Results using mass and economic allocations

The allocation rates are very different in both cases. There are no physical relationships depicting the share of GHG emissions between the heat released during reaction and the mass of sulphuric acid. Neither mass nor economic relation does so. Economic relation is more appropriate in cases of reporting as it better represents the motivation for heat recovery, although it may not serve as encouragement.

Conclusion

While using system expansion seems the best option, the outcome of the study is different if the substitution is done based on heat from hard coal or natural gas. This may not always be known, especially if the comparison applies to future plans. System expansion renders a negative footprint that is difficult to assess if reporting is the objective of the measurement.

System expansion is regarded as the best option for comparative assertions while economic allocation is better suited for reporting. In the first case, a sensitivity analysis is recommended on the substitution option.

Example – Caprolactam production

Authors: Henk Bosch (DSM), Sreepadaraj Karanam (SABIC)

Process description

In common processes for the production of caprolactam, there is a co-product stream of up to 4.5 kg ammonium sulphate per kg of caprolactam.

Allocation decision hierarchy

1) **Is it possible to subdivide the process into several and distinct processes to avoid allocation?**
No, ammonium sulphate is produced in the same reactions as the caprolactam. Only the crystallisation of the ammonium sulphate from the crude solution can be separated out.

2) **Is the system delivering co-product(s) that can be replaced by easily identifiable conventional product(s)?**
Yes, ammonium sulphate is used as fertiliser, and most ammonium sulphate that is not a co-product of organic synthesis is produced by the neutralisation of ammonia and sulphuric acid.

   Decision = Use system expansion

   Economic and mass allocation can be studied as sensitivity analysis.

Results (with illustrative values for allocation method parameters)

Method	Caprolactam	Ammonium sulphate	Environmental impact of caprolactam	Environmental impact of ammonium sulphate
System expansion	1 t	4.5 t	76%	24%
Mass	1 t	4.5 t	18%	82%
Economic (sales price)	2,500 €/t	180 €/t	76%	24%

Table 4: Results (with illustrative values for allocation method parameters)

Conclusion

In this example, there is a clear preference for system expansion, which is also applied by PlasticsEurope in their caprolactam eco-profile. Mass allocation would give a totally different result that would not represent the fact that this process is executed to produce caprolactam and not ammonium sulphate. The economic value of the ammonium sulphate confirms the assumption that it is an unintentional by-product. The price set selected for economic allocation coincidentally gives the same result that is obtained by system expansion.

Example – Cumene process

Authors: Henk Bosch (DSM), Sreepadaraj Karanam (SABIC)

Process description

The cumene process converts benzene and propylene into cumene, which is further converted into phenol and acetone. Phenol is the main product, and acetone is a major co-product. Almost the total global acetone demand in the world is fulfilled by this process. Acetophenone is a minor co-product generated in a side reaction in the last step. It is also recovered and sold. In this example, it is assumed that the molar ratio of production of phenol, acetone and acetophenone is 99:99:1. This is close enough to reality to be valid.

Allocation decision hierarchy

1) **Is it possible to subdivide the process into several and distinct processes to avoid allocation?**

   No, the three products originate from the same intermediate. Only the final recovery and purification steps for acetone and acetophenone can be separated out.

2) **Is the system delivering co-product(s) that can be replaced by easily identifiable conventional product(s)?**

   No, acetophenone is only produced commercially with this process. Acetone was formerly also produced by the dehydrogenation of isopropanol, but that route is hardly used anymore. Therefore, system expansion by substitution of an alternate manufacturing process for acetone would not be appropriate.

   Decision = Allocation is required

3) **Use the allocation based on the parameter describing the best underlying relations between the co-products as the main scenario.**

   The objective of the process is to produce phenol. Acetone is an essential co-product formed in equimolar amounts. Acetophenone (and CO_2) is generated instead of phenol and acetone in a parallel reaction in the last step. Because acetophenone is a valuable product, it is distilled from the residue after the recovery of phenol and acetone.

   Simple mass-based allocation for all three co-products is easy to perform, but it ignores the underlying relations mentioned above. Therefore a mixed method is more appropriate.

   Since the production of acetophenone is not the purpose of the process, the burdens of the process do not have to be allocated to it. However, the raw materials embodied in it and the specific burdens of the recovery (subdivision) to acetophenone do need to be allocated. The remainder of the burden has to be split between acetone and phenol.

The combination of the production of cumene and its conversion to acetone and phenol is designed to selectively oxidise benzene and propylene into phenol and acetone. The carbon and hydrogen atoms in the phenol originate from benzene, and those in the acetone originate from propylene. Therefore it makes sense to allocate benzene production to phenol and propylene production to acetone. The oxygen molecule is split between acetone and phenol, so the burdens of the production of oxygen should be evenly distributed between the two. There is no such clear physical relation for the other burdens in the processes, so they are allocated by mass. The result is shown in the last row of table 5.

4) If market prices of the several co-products are available, do they differ by more than 20% (average market price over three years)?
Yes, prices are very different, although no reliable acetophenone price is available. The best source found suggests the price is close to US$ 2/lb. The consequences are included in table 5.

5) Perform at least two allocation methods as a sensitivity analysis: economic allocation and another allocation based on another parameter (not correlated to the previous two) such as mass, energy and stoichiometry, and present the results according to these methods in the conclusions of the study.
Economic and mass allocation can be studied using sensitivity analysis.

Results (with illustrative values for allocation method parameters)

All currency shown in US$

Allocation method	Phenol	Acetone	Acetophenone	Environmental impact of phenol	Environmental impact of acetone	Environmental impact of acetophenone
Economic (sales price)	$1.43/lb.	$0.80/lb.	$2/lb.	73%	25%	1.3%
Mass	100 kg	62 kg	1.3 kg	61%	38%	0.8%
Mixed	2.4 kg CO_2-eq/kg	2.0 kg CO_2-eq/kg	3.3 kg CO_2-eq/kg	66%	33%	0.9%

Table 5: Results (with illustrative values for allocation method parameters)

Conclusion

This example shows that a mixed method is the best choice because it maximises the use of subdivision and takes into account physical relations. Simple mass allocation and economic allocation are ruled out by the decision tree and give different results compared to the preferred method.

Example – Combined heat and power

Author: C. Jason Pierce (Eastman Chemical Company)

Process description

A chemical company operates a combined heat and power (CHP) process that combusts natural gas to co-produce both steam and electricity. The steam is produced at three different pressure levels for use in on-site chemical manufacturing processes. A portion of the electricity produced is used for on-site chemical manufacturing, while the remainder of the electricity is sold to the external grid. CHP operations in chemical plants are often over-designed to allow for operating flexibility, swings and future capacity. CHP results in significantly advantaged energy efficiency as compared to conventional single-cycle electricity production.

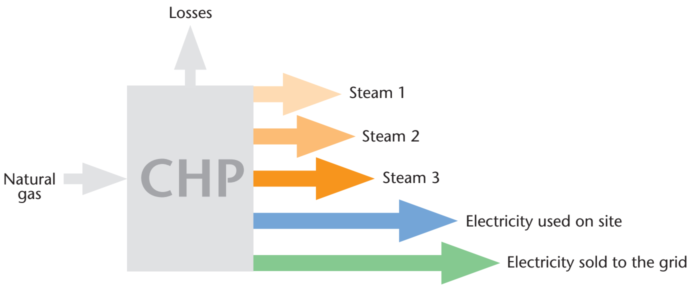


Figure 10: CHP process description

Allocation decision hierarchy

1) **Is it possible to subdivide the process into several and distinct processes to avoid allocation?**
No, the fuel combustion delivers two products (electricity and steam) simultaneously. Steam and electricity are different types of energy carriers.

2) **Is the system delivering co-product(s) that can be replaced by easily identifiable conventional product(s)?**
Yes, the electricity intended to be sold externally replaces grid electricity.

Decision = System expansion by substitution.

Electricity sold to the grid is interchangeable with commodity grid electricity (no renewable energy credits, etc.). The electricity sold to the external grid from CHP directly displaces electricity that would have otherwise been produced by energy utilities. The appropriate electricity grid mix for substitution should be carefully chosen.

System expansion is not applied to CHP electricity used on-site. All electricity directly used by the chemical plant should be based on supplier-specific data, which in this case is the CHP plant. For detailed supporting discussion see sections 8.1.1 and 8.5 of the PAS 2050:2011 standard.

3) **Use the allocation based on the parameter describing the best underlying relations between the co-products as the main scenario.**

After externally sold electricity is subtracted by system expansion, allocation is applied to the steam and internal electricity co-products. There are some challenges because the quality and functionality of each co-product is different. Three possibilities for the underlying physical relationship include energy, exergy (work potential) and the “efficiency method”. The *Guidance for Accounting and Reporting Corporate GHG Emissions in the Chemical Sector Value Chain* recommends the use of the efficiency method. Perhaps exergy is most closely related to the thermodynamic relationship between the different steam and energy products, yet it is a highly technical subject matter. For the sake of consistency with GHG Product Protocol and feasibility, it is recommended to use the efficiency method for allocations in CHP. A sensitivity study of all three allocation methods should be included.

See the following references:

- World Resources Institute/World Business Council for Sustainable Development (WRI/WBCSD). September 2006. *Allocation of Emissions from a Combined Heat and Power Plant.* Available at http://www.ghgprotocol.org/calculation-tools/all-tools
- WBCSD, 2013. *Guidance for Accounting and Reporting Corporate GHG Emissions in the Chemical Sector Value Chain.* Available at http://www.wbcsd.org/chemicals.aspx

4) **If market prices of the several co-products are available, do they differ by more than 20% (average market price over three years)?**

No, often not relevant. In most chemical plants the economic allocation is not fully relevant to CHP since there is not a market value for steam. Steam is an efficient energy carrier, but only within relatively short distances (very local energy), and is therefore often entirely used internally for heating and for directly powering some equipment.

5) Perform at least another allocation method as a sensitivity analysis using another parameter (not correlated to the first choice) such as mass, energy and stoichiometry, and present the results according to this method in the conclusions of the study.

With system expansion/substitution applied to externally sold electricity, a sensitivity analysis is performed to compare the footprint results according to the choice of allocation parameter.

Results

1. Natural gas (5,000 GJ input) was chosen as input fuel in the CHP process analysed.
2. Twenty percent of the electricity is sold externally. For sold electricity substitution, the "US: Electricity grid mix" data set from PE-GaBi 2012 database was used.
3. For efficiency method, the assumed efficiency is 35% for electricity and 80% for steam production.
4. For the exergy (work potential) allocation method, the calculations were based on the equations provided in the WBCSD CHP guidance document.

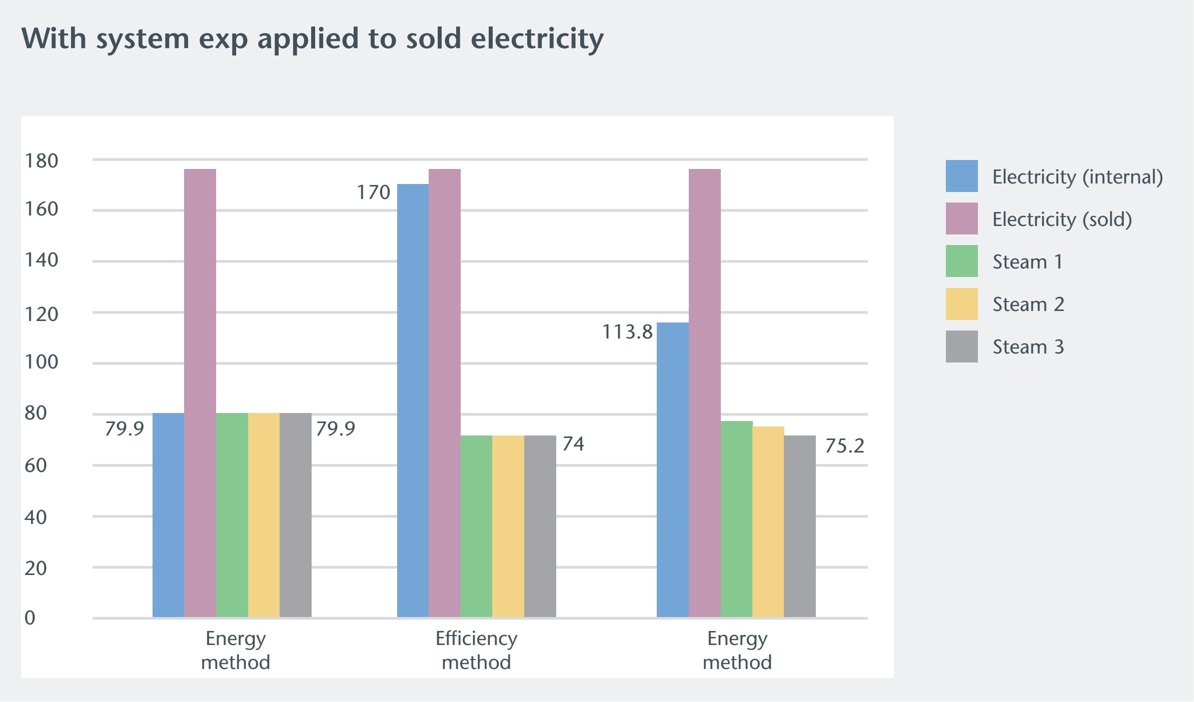


Figure 11 : Results with system expansion applied to sold electricity

Conclusion

It is recommended to **apply system expansion** to CHP electricity that is sold to the public grid.

After applying the system expansion, an efficiency method based on WRI/WBCSD guidance (2006) should be used to allocate the remaining inventory flows to steam and to electricity that is used internally within a chemical plant or sold directly to another entity. The energy method is not a fair representation of thermodynamic relationships. Depending on downstream uses of steam (i.e., heating versus mechanical work) it may be justifiable to use the exergy method rather than the efficiency method. In general, the efficiency method is recommended due to simplicity and alignment with *GHG Protocol: Guidance for Accounting & Reporting Corporate GHG Emissions in the Chemical Sector Value Chain. GHG Protocol for Chemical products.*

Example – Steam cracker

Authors: Ananda K. Sekar (SABIC), Sreepadaraj Karanam (SABIC), Gretchen Govoni (SABIC), Avantika Shastri (SABIC), C. Jason Pierce (Eastman Chemical Company), Henk Bosch (DSM)

Process description

Olefins are the primary intended products out of a steam cracker. However, these crackers also produce a range of co-product streams, all of which are utilised by the chemical industry. Table 6 presents an example of the range of co-products and their typical yields (on weight basis) for both ethane-based and naphtha-based crackers.

	Ethane	Naphtha
Ethylene	81	36
C_4 frac (58%)	0	10
Propylene	5	15
Py gas (30% is Benzene)	0	18
Fuel oil	0	4
H_2 rich gas (51%)	2	1
CH_4 rich gas	12	16
Total	100	100

Table 6: Typical yields of steam cracker products based on feedstock

As is evident, the composition of these co-product streams is very different for ethane- and naphtha-based crackers.

It is important to understand how steam cracking works. This process is based on the cracking of fossil hydrocarbons (predominantly ethane, LPG or naphtha) in large cracking furnaces that convert feedstocks to ethylene, propylene and other co-products. Coke formed from the process is subsequently cracked to form hydrogen and carbon monoxide. Acetylenes and diolefins are also produced as undesired (in most cases) by-products from this step. Post cracking, the products have to be fractionated. This is carried out using cryogenic fractionation, which involves a series of distillation columns.

The fractionation sequence is variable and several configurations are possible such as “front-end de-ethaniser” or “front-end depropaniser”, “demethaniser first”, etc. Acetylene hydrogenation can also be carried out before other separation steps or at the end of the separation sequence. Broadly, ethane based crackers rely on “front-end de-ethaniser” configurations since this allows separation of ethylene and ethane upfront, which form the majority of the product stream, from the rest of the product stream. This reduces traffic in downstream columns, which in turn, reduces capital costs.

Given this scenario, several allocation approaches are possible. However, the approach used here is based on the priority of allocation choices presented in Section 5.2.1.2. of the Life Cycle Metrics decision tree for allocation (reproduced as figure 12 later in this example).

Allocation decision hierarchy

1. Is it possible to sub-divide the process into several and distinct processes to avoid allocation?

As detailed in the previous paragraphs, cracker operations involve the following steps: cracking, compression and product separation. While all co-products share burdens of the cracking furnaces together, the separation section may have different burdens for each co-product depending on the sequence of separation. This would imply that only the product separation step may sanction different levels of environmental burdens to different co-products.

Unit process	Contribution to specific energy consumption	
	Share (%)	Estimated SEC (GJ/tonne)
Cracker	47%	11.0 GJ/t
Heat of reaction	23%	5.4 GJ/t
Dilution steam	6%	1.4 GJ/t
Heating+losses	18%	4.2 GJ/t
Compression	22%	5.2 GJ/t
Separation	31%	7.3 GJ/t
Chiller	21%	5.0 GJ/t
Condenser	16%	3.8 GJ/t
Ethane separator	5%	1.2 GJ/t
Steam	10%	2.3 GJ/t
Acetylene removal	3%	0.7 GJ/t
Heavy separation	7%	1.6 GJ/t
Specific energy consumption	100%	23.5 GJ/t

Table 7: Energy intensity of steam crackers*

**Source: Ernest Orlando Lawrence Berkeley National Laboratory (2000) report, available at http://www.energystar.gov/ia/business/industry/industrial_LBNL-44314.pdf*

As can be inferred from table 7, the separation step after steam cracking may contribute about 30% to the overall energy intensity of a cracker-based process, so its impact is significant.

When attempting to sub-divide the existing process into multiple sub-processes, the choice of the separation sequence (front-end de-ethaniser and front-end depropaniser) may have an influence on the burdens attributable to a specific product such as ethylene. De-ethaniser configurations may result in minimal load to ethylene (since ethylene is separated much earlier in the separation sequence), as compared to depropaniser configurations, which may apply higher burdens to the ethylene stream. It is important to note that these various configurations create bias on burdens to certain products versus others. The choice of feedstocks used for steam cracking strongly influences the product composition, hence the choice of desired separation scheme for optimum economic product separation. This may create a bias between burden applied to specific co-products.

Process data collection at this level of granularity may pose challenges. The subdivision of the process into distinct unit processes is not recommended in this case.

2. **Is the system delivering among other products/services either energy or fertiliser replacing an easily identifiable conventional product/service (e.g., petrochemical fertiliser or grid electricity, etc.)?**

   Steam cracking has been in practice for several decades with multiple feeds and configurations. Co-products produced via cracking have established value chains that would fall under conventional production routes for these co-products. Therefore, it cannot be claimed that these co-products displace a conventional product or service. Any credit for avoidance of conventional production cannot be applied for the cracker co-products.

3. **Is it possible to expand the system to other similar processes (only in the case of very specific and identifiable products/services)?**

   As previously detailed, some of the cracker products are sent back to co-located refineries (hydrogen, pyrolysis-gas, etc.) that supply the naphtha or other hydrocarbon feedstocks to the cracker. Certain other fractions (non-butadiene components of the C_4 fraction, for instance) are also recycled back to cracking furnaces to maximise the yield of desirable components. These streams, in principle, can be treated as recycle streams, and system expansion can be applied to discount this portion of the co-product stream from carrying any burdens of the process. Also, products such as BTX (benzene, toluene and xylenes) can be produced from the pygas stream, for which system expansion can be applied. However, aromatics separation and purification schemes are generally considered to be outside the boundaries of steam crackers, and system expansion is not applied to these co-products.

   However, in case of surplus energy from process off-gases that are exported outside the boundaries of the complex, system expansion can be applied to account for fuel offset credits.

   Decision = Allocation is required

4. **If market prices of the several co-products are available, do they differ by more than 20% (average market price over three years)?**

   Yes, market prices of the lowest and highest value products are typically more than 20% different, so this example will compare results using mass vs. economic allocation methods. First, consider economic allocation applied to just the main co-products (ethylene and propylene). The calculation of share of burdens is based on multiplying the mass fraction of each product (based on 1 kg total products basis) with the commercial value of the product (US$/kg) to get revenues per product (on 1 kg total products basis). Allocation is then based on share of revenues.

   As is evident from figure 10, economic allocation apportions 6%–7% percent higher burdens to propylene when compared to ethylene co-product. However, propylene prices have experienced significant price swings in the recent past. There may be instances when ethylene and propylene prices are comparable. There are also regional variations in these price trends (due to the local supply chain economics for natural gas and crude oil). Economic allocation may not appear to be a sensible choice for this case. It is also important to realise that the economic value of some of the other co-products (benzene, for instance) is at times comparable or even higher than that of the prime olefins. The following is an example that shows results from different allocation methods.

Results

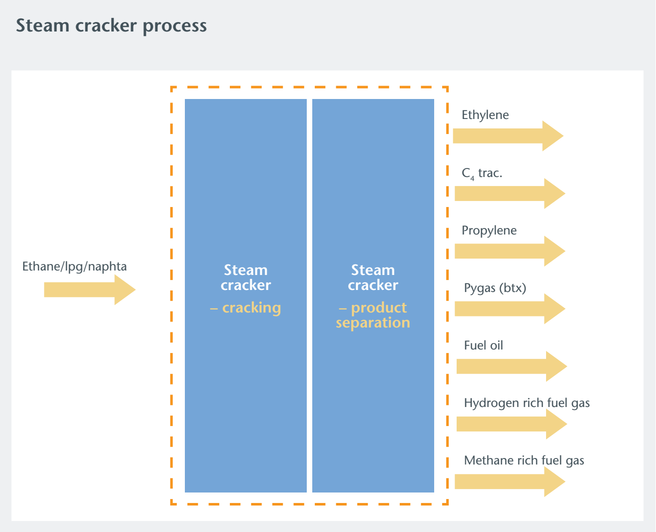


Figure 12: System description for steam cracker

Figure 12 illustrates a typical cracker and separation process. Depending on choice of allocation, as well as on cracker configurations, some of the co-products may be consumed as an internal fuel. These choices are documented for clarity. Table 8 presents the comparison of burdens attributable to 1 kg of ethylene and propylene based on various allocation approaches.

Mass, all products: All co-products are considered to share burdens of the process based on mass fractions of product slate. The off-gases (methane and hydrogen rich gases) and fuel oil are not assumed to substitute the ,on-site energy requirement.

Mass, HVC (high-value chemicals): Hydrogen fraction of hydrogen-rich off-gas is treated as a co-product. The remaining fuel streams (methane-rich off-gas and fuel oil) are assumed to be available for on-site energy needs. Fuel credit is applied based on their energy content.

Mass HVC allocation methodology is based on approaches used by PlasticsEurope and other references listed later in the text. This is based on the inclusion of select streams of co-products for allocation as described below:

(i) Only benzene portion of pygas, which constitutes 30% by weight (on an average), is included, whereas xylene and toluene are omitted;

(ii) Only hydrogen mass fraction of hydrogen-rich off-gas is included (which constitutes 51 percent by weight on average);

(iii) Only butadiene mass fraction of C_4 fraction is included (which constitutes 58 percent by weight on average). This may be an acceptable approach since the rest of the C_4 fraction is often recycled back to the cracking furnaces to maximise other desirable components. For clarity, the rest of the C_4 fraction would generally comprise isobutylene, mixed butenes and butane (commonly referred to as raffinate-1);

(iv) Methane-rich off-gas and fuel oil are omitted (since these streams are generally consumed internally as on-site fuels);

(v) Ethylene and propylene streams are included based on mass fraction of total product slate. This is also explained in table 8:

Final proposal for products to be distinguished The steam crack process belongs to NACE code 20.14 and the PRODCOM numbers of the marketable products (HVCs) are the following:	
Ethylene	20.14.11.30
Propylene	20.14.11.40
Butadiene (C_4 fraction)	20.14.11.65 (for butadiene), for the C_4 fraction there is not an own PRODCOM number, it falls in 20.14.11.(50-90) (acyclic hydrocarbons)
Benzene (aromatics)	20.14.12.23 (for benzene), the aromatics fall in number 20.14.12 (cyclic hydrocarbons)
Hydrogen (crack gas)	20.11.11.50 (for hydrogen), other crack gases fall in 20.14.11.20 (saturated acrylic hydrocarbons)

Table 8: Definition of HVC

Source: Methodology for the free allocation of emission allowances in the EU ETS post 2012 Sector report for the chemical industry *(2009), report by Ecofys and Fraunhofer*

Based on the above report, exclude the following operations from the cracking process (since these are considered to be part of downstream value chains and are not part of every steam cracker complex):

1. Hydrogen (pressure swing adsorption);
2. C_4 extraction;
3. Aromatics extraction;
4. Hydro-treating of pyrolysis gas.

There are various industry organisations that use the HVC approach for allocation to steam cracking co-products:

1. APPE;
2. PlasticsEurope;
3. BAT (BREF) – Best Available Techniques;
4. International Energy Agency (IEA);
5. Solomon Associates.

Mass, prime olefins: Herein, only ethylene and propylene are assumed to share the burdens. All fuel streams (hydrogen-rich and methane-rich off-gases and fuel oil, pygas) are assumed to be available for internal use. Fuel credit is applied based on their energy content.

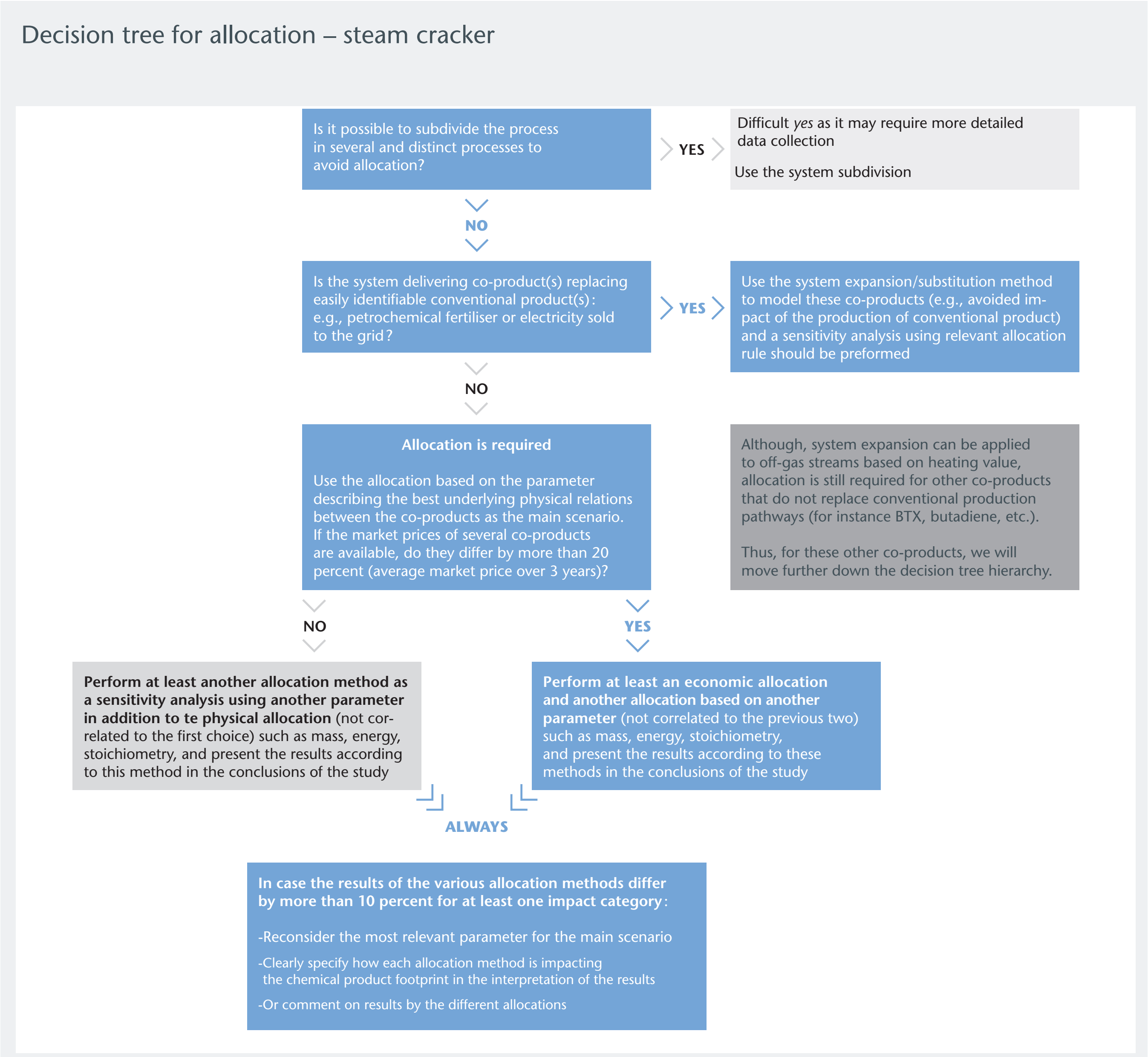
	Ethane (mass, all products)	Ethane (mass, HCV)	Ethane (mass, prime olefins)	Ethane (economic, prime olefins)	Naphta (mass, all products)	Naphta (mass, HCV)	Naphta (mass, prime olefins)	Naphta (economic, prime olefins)
Feedstock	100	100	100	100	100	100	100	100
	0	0	0	0				
Ethylene	81	81	81	81	36	36	36	36
C_4 frac (58%)	0	0	0	0	10	6	0	0
C_3+	5	5	5	5	0	0	0	0
Propylene	0	0	0	0	15	15	15	15
Py gas (30% is Benzene)	0	0	0	0	18	5	0	0
Fuel oil	0	0	0	0	4	0	0	0
H_2 rich gas (51%)	3	1	0	0	1	1	0	0
CH_4 rich gas	12	0	0	0	16	0	0	0
					0	0	0	0
Total mass of products sharing the burdens	100	87	86	86	100	63	51	51
Share of 100 units of impact per kg ethylene	1.00	1.15	1.17	1.16	1.00	1.59	1.97	1.90
Share of 100 units of impact per kg propylene	1.00	1.15	1.17	1.24	1.00	1.59	1.97	2.11

Ethylene @ US$ 1.17/kg NWE FD (May 2013)
Propylene @ US$ 1.33/kg NWE (May 2013)

Note: Fuel credits will be applied to all of the above figures

Table 9: Allocation scenarios for steam crackers

Decision tree for allocation



Is it possible to subdivide the process in several and distinct processes to avoid allocation?

Difficult *yes* as it may require more detailed data collection

Use the system subdivision

Is the system delivering co-product(s) replacing easily identifiable conventional product(s): e.g., petrochemical fertiliser or electricity sold to the grid?

Use the system expansion/substitution method to model these co-products (e.g., avoided impact of the production of conventional product) and a sensitivity analysis using relevant allocation rule should be preformed

Allocation is required

Use the allocation based on the parameter describing the best underlying physical relations between the co-products as the main scenario. If the market prices of several co-products are available, do they differ by more than 20 percent (average market price over 3 years)?

Although, system expansion can be applied to off-gas streams based on heating value, allocation is still required for other co-products that do not replace conventional production pathways (for instance BTX, butadiene, etc.).

Thus, for these other co-products, we will move further down the decision tree hierarchy.

Perform at least another allocation method as a sensitivity analysis using another parameter in addition to te physical allocation (not correlated to the first choice) such as mass, energy, stoichiometry, and present the results according to this method in the conclusions of the study

Perform at least an economic allocation and another allocation based on another parameter (not correlated to the previous two) such as mass, energy, stoichiometry, and present the results according to these methods in the conclusions of the study

In case the results of the various allocation methods differ by more than 10 percent for at least one impact category:

-Reconsider the most relevant parameter for the main scenario

-Clearly specify how each allocation method is impacting the chemical product footprint in the interpretation of the results

-Or comment on results by the different allocations

Figure 13: Decision tree for allocation – steam cracker

Conclusion

Based on this case study, "mass, HVC" (with system expansion for surplus off-gas credits) can be considered to be the best allocation approach for the steam cracking process. This approach ensures that all key intended co-products of the cracker are considered for allocation, while other by-products (which may either be recycled back to refineries or exported as energy streams) are covered by system expansion. This approach is gaining strong industry consensus, as shown by the list of adopters. However, as described in figure 12, it is recommended to perform other allocation approaches as part of sensitivity analysis, so as to highlight possible variations to the measured impacts based on each allocation approach being considered.

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8. Attribution of recycling benefits: The example of PET

Extracted and adapted from *Cradle-to-Gate Life Cycle Assessment of Valox iQ Resin and its comparison with Valox Resin*, final report, dated 16 November 2011, by Anju Baroth, Sreepadaraj Karanam, Gretchen Govoni, Hetal Dave and Dhaval Shah, SABIC Innovative Plastics

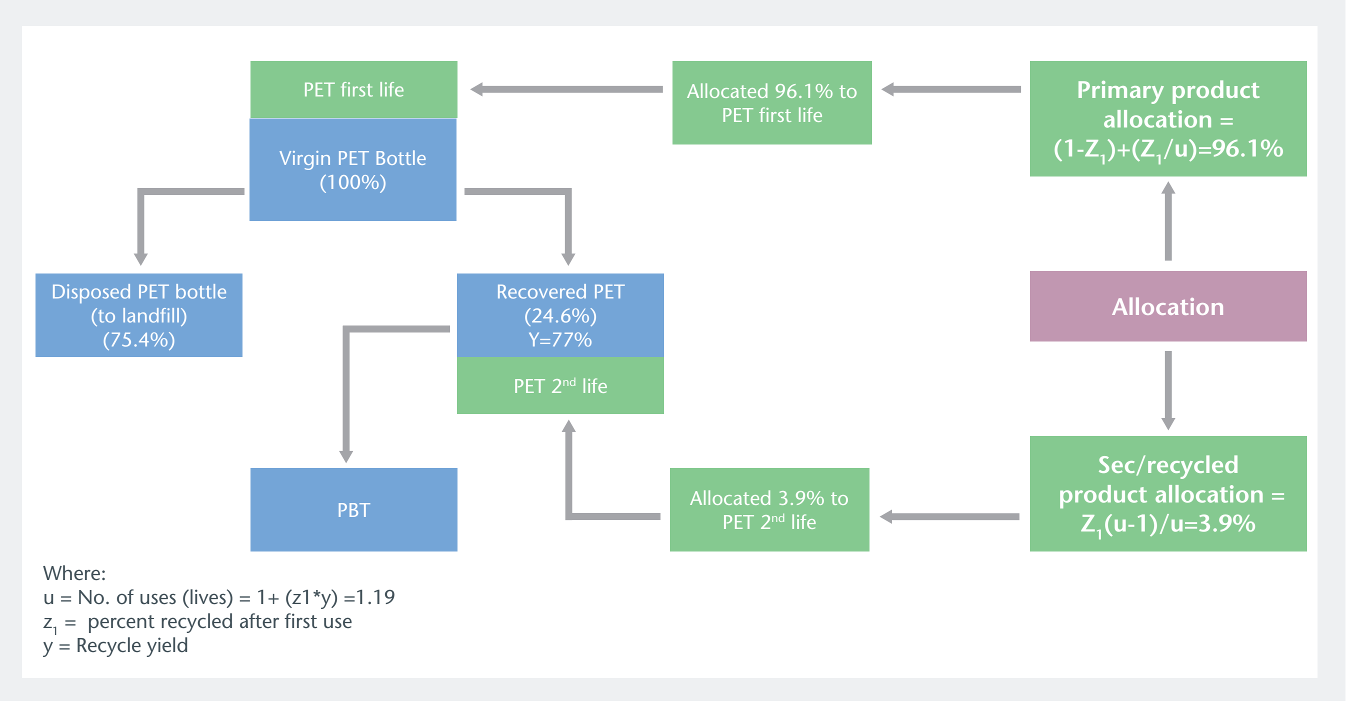
In recycling, allocation refers to how the environmental impacts from the recycled material are shared between the first life and each additional life. When material is used in one system and subsequently recovered, reprocessed, and used in another application, there are different methods that can be used to allocate environmental burdens among different useful lives of the material. Material production, recycling and disposal burdens can be allocated over all the useful lives of the material, or boundaries can be drawn between each successive useful life of the material. The following approaches can therefore be applied:

Cut-off approach

Under this approach, a boundary is drawn between the initial use of the material and subsequent recovery and recycling of the material. All virgin material production burdens are assigned to the first use of the material, and the burdens assigned to the recycled resin system begin with recovery of the post-consumer material. All of the burdens for material recovery, transport, separation and sorting, and reprocessing are assigned to the recycled material. The cut-off rule has been widely applied for recycled or recovered products. For example, in the ecoinvent database, heat recovered from waste incineration is considered free of environmental impact (Frischknecht et al. 2007a). Another example is EU Directive 2009/28/EC, in which crude glycerol is treated as waste and is considered to be free of greenhouse gas emissions. The cut-off method is considered simple and easy to apply because no data of the first life is needed.

Open-loop recycling allocation

In the open-loop allocation method, the burdens for virgin material production, recovery and recycling, and ultimate disposal of recycled material are shared among all the sequential useful lives of the material. Therefore, the share of virgin material burdens allocated to any individual use of the resin depends upon assumptions about the total number of useful lives of the resin. For example, a post-consumer, recycled bottle-grade – polyethylene terephthalate (PET) in this case – is used in a new process for manufacturing polybutylene terephthalate (PBT). Two useful lives of the material (resin used in a virgin product, then in a recycled product, then disposed) is considered. So the burdens for virgin material production, post-consumer recovery and reprocessing are divided between the virgin and recycled uses of the material. Hereafter a scheme represents this open-loop recycling allocation, based on the ISO 14049 method (section 8.3.3) for modelling open-loop recycling.



Where:
u = No. of uses (lives) = 1+ (z1*y) =1.19
z_1 = percent recycled after first use
y = Recycle yield

Figure 14: Recycling process and allocation of benefits for PET

50/50 approximation

The 50/50 approximation method is a market expansion model that considers the supply and demand for recycled PET. It asks how much demand for recycled PET is fulfilled by increased recovery/collection of PET (less being sent into the waste stream) and how much is fulfilled by someone else not having access to as much recycled PET as they could use, therefore forcing others to use more virgin PET. The 50/50 approximation assumes that 50% of demand comes from additional recovery of PET (less waste), and 50% comes from someone else using virgin PET instead of recycled PET. This method is called "approximation" because it is used when the actual supply and demand markets for recycled PET are unknown. The method is an approximation of a more precise calculation of the market using supply and demand price elasticity. In the absence of current price elasticity data, the 50/50 approximation is used. The value judgment credits the user of recycled material, but does not give full credit because of the assumption that there is only a limited supply of recycled material to be used.

Fully utilised and underutilised market for the recycled PET – market-based model for system expansion

The market-based model for system expansion considers whether the market for recycled PET is fully utilised or underutilised. It asks what happens to each of the involved processes when an extra unit of each product is demanded without a corresponding increase in the demand for the other product(s). A fully utilised market is one where the entire recycled PET quantity is consumed; an underutilised market is one where not all the recycled PET is consumed. The model states that in a fully utilised market, the use of additional recycled PET requires that more virgin PET must be produced. In this market situation, the supply of recycled PET is in some way constrained and no additional PET can be taken out of the waste stream to fulfil additional demand. In the fully utilised market, the product using the recycled PET takes the environmental burdens of the virgin PET, which must be produced to fulfil the additional market demand. The model states that in an underutilised market, the use of additional recycled PET will result in more PET being taken out of the waste stream. The product using the recycled PET takes the environmental credit for removing the PET wastes and takes the environmental burdens for refurbishing this waste into usable recycled PET. This model attempts to value both the manufacturer of recyclable products and the user of recycled material in proportion to market demand. While this appears to be the most "fair" way to allocate burdens, the results shift with the market because of volatility.

Economic allocation of the virgin PET environmental burdens based on an economic model

The economic approach to recycling considers the economic value of the total product stream (value of the virgin PET and the recycled PET) and makes the allocation based on this total value. Using a market price (for 2008, for example) for virgin PET set at US$ 0.70/lb. and the recycled PET set at US$ 0.24/lb., 93.8% percent of the environmental burdens of virgin PET were allocated to the first life and 6.1% were carried through to the second life. Like the market-based allocation, economic allocation values both the manufacturer of recyclable material and the user of recycled material. It also changes with the market. It is expected that the economic allocation reflects the market constraints, which makes the philosophy of the two methods similar.

Conclusion

From the above recycling allocation approaches, it is observed that each recycling model incorporates certain value judgments that affect the way environmental burdens are assigned between the lives of the material. The cut-off method builds on a value judgment that encourages the reuse of recycled materials, generating higher value for the recycled material, which may, in turn, increase the amount of collectable material. Open loop allocation, on the other hand, drives recycling as well as reuse by giving credit to recycler as well as recyclee. To expand the system boundary and allocate the burdens based on either the number of lives (open loop), the market expansion (50/50 approximation) or market-based model for system expansion requires assumptions about the market that may or may not be accurate and will shift with time. However, using any of the recycle allocation method choices (except the fully utilised scenario) results in the same conclusion, i.e., that producing PBT resin (from PET bottles) results in less total cradle-to-gate environmental burden than production of virgin PBT resin.

In any case, the default recommendation is to follow the consensus along the value chain if it has already defined its specific allocation method, and to perform sensitivity analyses if the preferred option deviated from the 50/50 approximation (which is the EU PEF recommendation).

9. Data management plan checklist (from GHG Protocol Product Life Cycle Accounting and Reporting Standard)

Component	Information	Rationale
Responsibilities	Name and contact details of persons responsible for: • Management of product inventory • Data collection for each process • Internal review or audit procedures • Assurance procedures	Ensures institutional knowledge is maintained and allows relevant person(s) to be identified as accountable for: • Confirming and checking information during any internal or external audit procedures • Producing consistent future product inventory
Product description	Description of the product and functional unit	Provides internal auditors, assurance providers and those doing future product inventories with information on the product/functional unit
Inventory boundary	• Inventory boundary description (e.g., cradle-to-grave or cradle-to-gate) • How the boundary was derived • Attributable processes included in the inventory • Attributable processes excluded from the inventory (including rationale for exclusion) • Information on how the product use and end-of-life profile was determined	Provides internal auditors, assurance providers, and those doing future product inventories with sufficient information to understand and replicate boundary decisions
Allocation	Allocation methodologies used and where they were used	Provides internal auditors, assurance providers, and those doing future product inventories with sufficient information to understand and replicate allocation decisions
Data summary	• Data collection procedures, including data sources for each process	Records all data sources and allows others to locate data sources (for audit or future product inventories). Also provides information on which suppliers have been approached for data
	• How data quality assessment and uncertainty assessment were undertaken	Enables data quality to be tracked over time and improved
	• Data sources where better quality data is preferable and plan for how to improve that data	Identifies where data sources should be improved over time (e.g., needed emissions for laptop computer but could only obtain desktop computer information), including those suppliers who were asked to provide data and those who were not
	• Criteria used to determine when an inventory is to be re-evaluated, including the relevant information, changes to the system to be tracked over time, and how these changes should be tracked	Allows data and information sources to be tracked and compared over time. It may also involve identifying a system (e.g., document tracking and identification system) to ensure data and information are easily located and under what conditions they were used or collected
	• Calculation methodologies used (and references). This includes documenting where the calculation methodology for any data used was not available.	Provides internal auditors, assurance providers and those doing future product inventories with details on how emissions were calculated
Inventory results calculations	• Calculation methodologies and changes in methodologies over time	Allows for easier baseline recalculation when tracking inventory improvements
	• Global warming potential (GWP) values used	Allows for consistency over time
Performance tracking	When tracking performance, details of the base inventory adjustment policy	Prescribes clearly a trigger for adjusting a base inventory enabling tracking of performance over time
Data storage procedures	• How and where data is stored	Allows information to be easily located
	• Length of time data is to be archived	Keeps a record of how long information is stored to prevent searches for information that is no longer kept
	• Backup procedures	Ensures backup procedures are implemented
Quality assurance/quality control (QA/QC) procedures	• Assurance and control procedures	Ensures adequate processes are in place to check data collection, input and handling, data documentation and emissions calculations

10. Comparison of requirements with other standards

Colour code

🟨	Fewer requirements than other guidance
⬜	Alignment with *Life Cycle Metrics for Chemical Products* guidance
🟩	*Life Cycle Metrics for Chemical Products* guidance goes beyond
🟧	Conflict with *Life Cycle Metrics for Chemical Products* guidance

Topics		Life Cycle Metrics for Chemical Products guidance specific requirements	EU PEF	ILCD Handbook	ISO 14040:2006 and 14044:2006	GHG Product Protocol	GHG Protocol scope 3	Avoided emissions
Modelling approach	Multi-criteria analysis		⬜	⬜	⬜	🟩	🟩	🟩
	Attributional versus consequential	This guideline is meant for the calculation of product footprints in an attributional way. Consequential studies, which are useful to assess changes in environmental flows due to decisions, are out of the scope of this guideline. Consequential studies obey different principles and therefore would need a guideline of their own.	🟨 Both attributional and consequential approaches	⬜ Attributional approach	🟨 No distinction between attributional and consequential approaches	⬜ Attributional approach	⬜ Attributional approach	⬜ Attributional approach
Education		Various additional examples and recommendations relevant for chemical products.	🟩	🟩	🟩	🟩	🟩	🟩
ISO 14040:2006 and 14044:2006		Chemical product footprint studies shall be based on the ISO 14040:2006 and 14044:2006 requirements as much as feasible. All deviations shall be explained and documented in the product footprint report.	⬜	⬜	⬜	⬜	⬜	⬜
Goal and scope		The following specific requirements are to be taken into account for a chemical product footprint study goal definition in compliance with ISO 14040:2006 and ISO 14044:2006. The chemical product footprint study report shall: - State the intended application(s) of the [chemical product footprint] results in a precise and unambiguous way (*ILCD Handbook*); - Explain the reasons for carrying out the [chemical product footprint] study, name the drivers and motivations, and especially identify the decision-context (*ILCD Handbook*); - State clearly the business goal (GHG Product Protocol); - Identify the target audience of the study, i.e., to whom the results of the study are intended to be communicated (*ILCD Handbook*).	⬜	⬜	⬜	⬜	⬜	⬜

System boundary	Cradle-to-grave versus cradle-to-gate	Chemical product footprint system boundaries should be "cradle-to-grave". In case of a cradle-to-gate chemical product footprint, boundaries shall include end-of-life for all waste streams generated during the production of the product. Boundaries should be set such that all inventory inputs and outputs (except for the studied product) are reduced to elementary flows.	🟩	The study shall include all activities from cradle-to-grave.	The study shall include all activities from cradle-to-grave.	🟩	The study shall include all activities from cradle-to-grave.	The study shall include all activities from cradle-to-grave.
	Precise prescriptions in case of cradle-to-gate	In the case of a cradle-to-gate chemical product footprint study, a specific limitation statement shall be included in the chemical product footprint study report in order to inform the reader that comparability of the cradle-to-gate chemical product footprint with other products may not be relevant and may lead to incorrect conclusions because of differences in downstream impacts. GHG emissions generated from the chemical product will be different between the cases of incineration and landfill of the end product. The following cradle-to-gate footprints may be compared with chemical and functional equivalents in a given application. For example, polypropylene issued from different processes, such as i) the cracking of naphtha or other liquids or ii) the cracking of butane or propane. The chemical product footprint life cycle steps taken into account shall be clearly listed and described in the chemical product footprint study. Any step exclusion shall be justified.	🟩	The study shall include all activities from cradle-to-grave.	The study shall include all activities from cradle-to-grave.	🟩	The study shall include all activities from cradle-to-grave.	The study shall include all activities from cradle-to-grave.
Functional unit	Reference flow	From GHG protocols		🟩	🟩			
	Function unit definition	The functional unit shall be consistent with the goal and scope of the study.	🟩			🟩	🟩	🟩
		As the functional unit specifies the benefit provided to the customer, the functional unit shall be equivalent for all compared solutions. To ensure products in a comparative chemical product footprint study are exchangeable in the selected market, relevant quality criteria shall be taken into consideration. The following three quality properties shall be used to assess whether compared solutions are truly exchangeable: - Functionality, related to the main function of the solution; - Technical quality, such as stability, durability, ease of maintenance; - Additional functions rendered during use and disposal.. For cradle-to-grave studies, companies shall specify the duration of the functional unit, i.e., for how long the performance of the final product or service needs to be maintained. The chemical product footprint report shall explain how this duration has been determined in relation to the lifetime of the product.		🟩	🟩			
	Lifetime and service life	Both duration of the functional unit and lifetime of the product should be in line with standards used in the market (e.g., product category rules, studies from reputable organisations and studies by leading companies in the value chain).		🟩	🟩	🟩	🟩	

Impact categories and methods	Materiality guidance to identify the communication requirements	The following impact categories shall be reported in the chemical product footprint study report: - Global warming; - Photochemical ozone formation; - Air acidification; - Resource depletion (fossil fuels); - Abiotic depletion (element); - Eutrophication (marine and freshwater); - Human toxicity and eco-toxicity. The following impact categories should be addressed in the chemical product footprint study report: - Dust and particulate matter; - Land quality and species richness (in case of communication, should communicate on both). The following impact categories may be addressed in the chemical product footprint study report: - Ozone depletion; - Water scarcity.						
Impact assessment methods	Impact category indicators and characterisation models (see section 4.5.1).	- Worldwide and regional requirements. - Updates according to latest available methodological best practices for chemical products.	- World Meteorological Organization characterisation source years, which have been updated. - Kg ethylene eq. impact category indicator for photochemical ozone formation have been preferred to kg non methanic volatile organic compounds eq., since kg NMVOC could result in addition of gases with different characterisation factors. - The impact categories above mentioned for which regional specificities have a high impact and for which Lime 2 model is recommended for Japan.					

Elementary and intermediate flows	Additional methodological guidance on LHV for CED	The following intermediate flows shall be addressed in the chemical product footprint study report: - Cumulative energy demand (CED); - Renewable energy consumption; - Non-renewable energy consumption. CED and renewable/non-renewable energy consumption shall be assessed using the fuel's lower heating values (LHV).						
	Additional methodological guidance on water	Water consumption, including water consumption of upstream raw materials, should be disclosed and account for the whole system boundaries. When water consumption is disclosed, the chemical footprint report shall include at least cradle-to-gate water consumption according to the following categories: surface freshwater, renewable groundwater and fossil/deep groundwater. In addition, cradle-to-gate water consumption of seawater should also be disclosed if relevant. The sum of all consumption from these compartments should cover all water consumption for chemical product production (see section on cut-off).						
	Additional methodological guidance on land occupation	Land occupation intermediary flow may be assessed and disclosed in the chemical product environmental footprint. If disclosed, this indicator should be accounted in m^2a unit (area in square meters*year). The following land categories may be used for classification (ecoinvent): - occupation urban - occupation, industrial area - occupation, traffic area - occupation, mineral extraction site - occupation, dump site - occupation, arable - occupation, arable, monotone-intensive - occupation, arable, non-irrigated organic - occupation, permanent crop - occupation, pasture and meadow - occupation, forest - occupation, shrub land - occupation, water areas Land transformation (m^2) may be considered as well for reporting.						
	Additional requirements on waste	For cradle-to-gate studies: The waste tonnages may be disclosed according to the following categories: - Hazardous waste disposed; - Non-hazardous waste disposed; - Radioactive waste disposed. When waste flows are disclosed, all types of disposed waste (landfill and incineration without energy recovery) should be accounted. Wastes are intermediary flows in a product system, exchanged between the unit process that generates them and the one(s) that treat them. Accounting for them should not stop/prevent the practitioner from including the treatment process and the associated burdens since these are part of the cradle-to-grave life cycle and even cradle-to-gate life cycle for the production wastes. For cradle-to-grave studies: When waste flow is disclosed, all waste generation during the life cycle of the product shall be accounted. The tonnages may be disclosed according to the same categories as cradle-to-gate studies. In that case, all types of disposed waste (landfill and incinerated) should be accounted.						

Data sources requirements and quality management	Use of the pedigree matrix	The most accurate and available primary data shall be used. Any use of secondary data when primary data is available shall be justified using the pedigree matrix.	🟩	🟩	🟩	🟩	🟩	🟩
	Specific requirements on primary data for chemical products	The most accurate available data shall be used for primary data. The following on site measurements should be used in priority when data is available and accurate: - Aggregation of registered measures for consumptions (water, energy, raw material); - Continuous measurements for air and water emissions (if not available: spot measurements may be used).	🟩	🟩	🟩	🟩	🟩	🟩
	Choice of secondary source based on quality	Quality of secondary data (including supplier data) shall be assessed according to the criteria specified in section 4.6.2.	🟩	🟩	🟩	🟩	🟩	🟩
	Detailed recommendations by source	The sources of secondary data to be used should be based on the quality assessment results, from the following list of source categories detailed in section 5.1.2.1. (see also additional requirements per data source in this section).	🟩	🟩	🟩	🟩	🟩	🟩
	Transparency	For all secondary data, specific attention has to be paid to the methodological hypothesis behind these data sets and such assumptions shall be carefully acknowledged by the practitioner before using the data. Allocation approaches used (if any), cut-off, data gaps (lack of or incompleteness of emissions data, etc.) should be mentioned.			🟩	🟩	🟩	🟩
	Electricity	Recommendations from section 5.1.2.1. adapted from and in line with the European PEF shall be applied for electricity.		🟩	🟩	🟩	🟩	🟩
	Data quality assessment	Data quality indicators: The following five indicators shall be used to assess the quality of the data (both specific and generic) used for the modelling: reliability, completeness, time representativeness, geographical representativeness and technological representativeness. Scoring: The data quality scoring shall be assessed according to the pedigree table from ecoinvent (Data Quality Guideline from the ecoinvent database version 3, modified from Weidema, 1998). This table describes the quality level scoring (from 1 to 5) for each criterion. The assessment and rating on data quality should be performed for each unit process with a significant contribution (>10 percent) to at least one environmental impact. The results should then be aggregated at the life cycle stage level.			🟩			
	Data management plan	The data used for chemical product footprint shall be managed according to the GHG Product Protocol Data Management Plan Checklist (see Appendix 10).	🟩	🟩	🟩			🟩

Cut-off	- Mandatory assessment of mass and energy of non-accounted components in case of cut-off - Additional requirements on elements to include in the scope of the study	Environmental significance shall be assessed as defined by ISO 14040:2006 and 14044:2006 based on expected emissions. See example below for materiality of non-accounted toxic compounds. All mass, energy elementary flows should be accounted. If not, the chemical product footprint study report shall include the estimation of completeness, based on: - Mass cut-off (in percent of total system input mass): best estimation of the mass all non-accounted components of the product; - Energy cut-off (in percent of total energy consumption): estimation of all energy consumption (cumulative energy demand) of non-accounted mass inputs. Unless expected to be material, the following elements should be excluded from the scope of the chemical product footprint study: - Business travel (according to the GHG Protocol scope 3 definition); - Employee commuting (according to the GHG Protocol scope 3 definition); - Investments (according to the GHG Protocol scope 3 definition); - Infrastructure life cycle impacts; - Energy consumption and goods not directly related to the product production. For example, recreation facilities, canteen, administration and R&D related impact. In case it is not feasible to apply these exclusions (in particular if data sets do not allow it), a statement should be included in the data quality section of the chemical product footprint report.	Cut-off not allowed	🟩	🟩	🟩	🟩	🟩
Allocation rules	New decision tree for allocations, involving sensitivity analysis	When a system is delivering several products with different functions, the decision tree from section 5.2.1.2. shall be used to choose the method to calculate the environmental impacts of each product.	🟩	🟩	🟩	🟩	🟩	🟩
Recycling		When a consensus along the value chain has already defined its specific allocation method (corrugated board, steel, aluminium cf. Appendix 6 - LCI data sets - Industry average eco-profiles published by industry associations) this attribution method should be used. In other cases, recycling should be accounted as described in the EU PEF, using the 50/50 attribution method: “the formula provided […] allocates impacts and benefits due to recycling equally between the producer using recycled material and the producer producing a recycled product: 50/50 allocation split” (EU PEF). Whatever the choices made on the attribution of recycling impacts/ benefit: - The results shall be communicated both with the total amount of impacts and including the recycling credit attribution. - A sensitivity analysis shall be performed using the EU PEF 50/50 method.		🟩	🟩	🟩	🟩	🟩

Avoided emissions		When comparing alternative solutions within the chemical industry value chain, avoided emissions shall be accounted and attributed as specified in the *Guidance on Accounting and Reporting Avoided Greenhouse Gas Emissions in the Chemical Industry* – Draft – October 2013.	🟩	🟩	🟩	🟩	🟩	⬜
Biogenic uptake and emissions	Specifications on end-of-life CO_2 credit	Separate accounting and reporting shall be performed for fossil and bio-based carbon emissions and the carbon stored in the raw biomass shall also be quantified. For cradle-to-gate, a carbon credit appears as a negative value due to a CO_2 eq. uptake during the growing phase of the plant at the origin of the renewable material. The fate of this bio-based carbon content in the product depends on the end-of-life of the final product and therefore often leads to a neutral balance due to the release of the bio-based carbon at the end-of-life (in case of incineration for instance). In such a case, the end-of-life of the product and its impact on the carbon elementary flow balance shall be at least qualitatively described in the chemical product footprint report.	🟩	🟩	🟩	🟩	🟩	🟩
Carbon storage and delayed emissions		The sensitivity of carbon credits associated with temporary carbon storage or delayed emissions should be assessed, and therefore the sensitivity should be discussed when interpreting the global warming impact results. When being communicated, carbon delayed emissions shall be reported separately. For more information on temporary carbon storage and the way to assess delayed emissions, please refer to the ISO/TS 14067:2013.	🟩	Excluded from the usual scope of study. However, if included because part of the goal of study, the ILCD Handbook provides detailed operational guidance.	🟩	Carbon that is not released as a result of end-of-life treatment over the time period of the study is treated as stored carbon. The time period should be based on science insofar as possible, or be a minimum of 100 years. Delayed emissions or weighting factors (e.g., temporary carbon) shall not be included in the inventory results, but can be reported separately.	🟧	🟩
Direct land-use change/ indirect land-use change		Greenhouse gas emissions that occur as a result of indirect land-use change should not be considered. Greenhouse gas emissions from direct land-use change shall be allocated to goods or services for 20 years after the change occurs using the IPCC default values table from section 5.2.6. (IPCC updates of this table should be used in priority if available.)	⬜	⬜	🟩	Additional guidance provided for calculation.	🟨	🟩

11. Areas of concern and call to action for scientific, LCI database and LCA software development communities regarding life cycle impact assessment and results interpretation

The present document is one of the outcomes of a collaborative process among 10 global chemical companies and members of the WBCSD, with the support of PricewaterhouseCoopers. The objective of this working group is to ensure the consistent and credible communication of product environmental footprints by the chemical sector, partly through the creation of a global framework to align life cycle metrics. The result is *Life Cycle Metrics for Chemical Products: A guideline by the chemical sector to assess and report on the environmental footprint of products*. In drafting this guidance, the working group noted several areas of concern, summarised here, and suggests a call to action for other life cycle assessments and for practitioners.

Difficulty in dealing with regional specificities (especially for air acidification, resources depletion, water and toxicity)

The chemical industry is part of a complex global supply chain. Feedstocks, intermediates and finished goods are produced and transported across diverse geographies. Impacts such as acidification, resource depletion, water availability and quality, and human/eco-toxicity are localised in nature. For example, local weather patterns and population densities strongly influence the transport and fate of and human exposure to toxic material releases. Generalised models have limited usefulness for decision-making due to the lack of granularity of impact categories that are local in nature.

Call to action

1. Regionalize individual flows and inventories in life cycle assessment (LCA) software and LCI databases to allow regionalised impact assessment (for each model or inventory flow, add location specifications to state where consumptions and emissions occur).
2. Develop and operationalize regionalised characterisation factors for the preferred impact assessment methods.
3. The effort to extend LCI databases (such as ecoinvent) to all regions of the world should be accelerated. In particular, LCI data is needed from major manufacturing regions such as China, India and Brazil. A common methodology needs to be applied across all regions.

Gaps in human toxicity and eco-toxicity impact methods assessment

The chemical industry is very serious about risk assessment and safe use of the products it produces. Key industry initiatives such as Responsible Care and the International Council of Chemical Associations (ICCA) Global Product Strategy are complementary to important regulatory efforts such as REACH (Registration, Evaluation, Authorization and Restriction of Chemicals). Risk assessment and industrial hygiene efforts have been ongoing and continually improving for decades. The assessment of human and ecotoxicity impacts across the full life cycle is a challenging and relatively new undertaking, and chemical companies should be supportive of assessing and appropriately minimising life cycle impacts of chemical products.

It is commonly agreed that toxicity is important. However, most of the time toxicity data is not reported in environmental product declarations. Therefore, methods (such as USEtox) considered by the chemical industry should be:

- Understandable;
- Back-traceable; and
- Reliable.

The development of the USEtox model through a consensus process was a significant step towards a useful characterization model. However, many companies are not supportive of reporting human and ecotoxicity life cycle inventory assessment (LCIA) impacts (from USEtox or other methods) for a variety of reasons. Some of the key factors limiting the widespread acceptance of USEtox are as follows:

- Data limitations
  1. USEtox version 1.01 contains 3,073 organic substances, but 1,818 of the substances are flagged to indicate an issue with the data. Only 1,255 substances are unflagged. LCA software such as GaBi only includes the unflagged substances. This leaves a tremendous number of substances unaddressed by the existing method. Many real-world commercial chemical substances are not included. See examples of substances not covered in USEtox in addendum A.
  2. Inorganics are likewise inadequately covered. Generic particulate matter (less than 10 microns) does not appear to be included either.
  3. Eco-tox characterization factors are only available for freshwater (not soil or seawater).
  4. Reliability for decision-making is questionable for some substances. For instance, the USEtox characterization of methanol appears implausible compared to methymetacrylate (MMA).

5. Total human health effect factor MMA = 0,080444 [cases/kg intake] and methanol = 0,001017 [cases/kg intake].
6. Methanol, however seems to be generally more toxic and hazardous than MMA according to Globally Harmonized System (GHS) hazard communication labels (see below).

Methanol

Methylmethacrylat

- Documentation and traceability
  1. The official mechanism for adding new substances to USEtox is not clear.
  2. Limited information on primary literature is provided, making it virtually impossible to track USEtox data back to primary sources. (As a suggestion, perhaps this could be organised on demand through a USEtox blog.) Some information on source hierarchy is discussed in the user manuals, but it is important to know the actual sources for individual substances.
- Lack of regionalisation
  1. As previously discussed, toxicity often has a local impact – particularly with regard to transport, fate, exposure and uptake. Commercial products and intermediates are produced globally in a distributed manner. USEtox is currently implemented in major LCA software using a generalised model with low spatial resolution.
- Transparency and quality of data
  1. There does not appear to be a quality assurance process for data included in USEtox. The mechanism for flagging, reviewing and amending questionable data in USEtox is not clear. A peer group of expert toxicologists should be involved in such activities to provide proper assessment and interpretation of source data, exposure parameters, etc.
- Uncertainty
  1. The reported uncertainty[12] of USEtox is up to several orders of magnitude higher than other common impact assessment categories (such as global warming potential). This creates challenges with proper interpretation.
  2. For such LCIA information to be broadly reported, there needs to be an improvement in the assessment and communication of the inherent uncertainty. (One suggestion is to consider reporting toxicity impacts on a logarithmic scale.)

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[12] Rosenbaum et al. 2008. "USEtox—the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment". *International Journal of Life Cycle Assessment* 13:532-546.

Call to action for USEtox

1. Add a quality assurance process and a mechanism for adding new substances.
2. Continue to expand the substance database.
3. Provide source data references for substances.
4. Implement regionality.
5. Develop enhanced tools for uncertainty analysis and work to reduce uncertainty.

Difficulties in applying water footprint methods and tools for product assessment

Efforts are currently being made in this area. Challenges include:

- Lack of regionalised inventory data;
- Lack of differentiation between usage and consumption in inventory data;
- Inconsistency in methodology within secondary data sets and databases;
- Lack of commonly used and software implemented LCIA methods;
- Importance of assessing water impacts and not just inventories.

Call to action

1. Develop uniform methodologies and implement them in standard LCA tools.
2. Differentiate individual flows and inventories in LCA software and LCI databases to account for regionality and types of water use and consumption (see also above with the regionalisation).

Inconsistencies between different characterisation methods or software in which the methods are implemented

Key challenges in assessing environmental impact of products using different software include:

- Availability of updated impact assessment methods;
- Discrepancies due to nomenclature issues or decisions regarding parsing grouped emissions (e.g., PM10 into PM2.5 and PM2.6-PM10, or treatment of "metal compounds");
- Differences in characterisation factors for key substances and key methods.

An analysis presenting gaps and inconsistencies of an example assessment using different life cycle impact assessment methods and software is presented in addendum B.

Call to action

Harmonise practices linked to the implementation of impact assessment within LCA software

Inconsistent quality or scope of available databases

- Need for more high-quality and regionalized data.
- Need for better documentation of data sources, assumptions and system boundaries in databases.
- Need for clearer, more transparent and consistent data uncertainty treatment and quality indication across all LCA software.
- Regionalized LCI data is lacking, as previously discussed (notably from China, Brazil and India).
- Procedural instructions regarding how to best deal with unavailable data.

Addendum A – Examples of substances not included in USEtox

N° CAS	Flow not included in USETox
	SOx
	NOx
100728-84-5	imazamethabenz
104098-48-8	imazapic
109293-97-2	diflufenzopyr
112143-82-5	triazamate
122453-73-0	chlorfenapyr
131983-72-7	triticonazole
139001-49-3	profoxydim
139968-49-3	metaflumizone
142469-14-5	tritosulfuron
149961-52-4	dimoxystrobin
163515-14-8	dimethenamid-P
175013-18-0	pyraclostrobin
1779-81-3	aminothiazoline
188425-85-6	boscalid
210631-68-8	topramezone
220899-03-6	metrafenone
248593-16-0	orysastrobin
372137-35-4	saflufenacil (BAS 800 H)
50-00-0	formaldehyde
58667-63-3	flamprop-M
630-08-0	carbon monoxide
7440-50-8	copper compounds
7704-34-9	sulphur
85916-84-3	mercaptazole
865318-97-4	ametoctradin (BAS 650 F)
87818-31-3	cinmethylin
907204-31-3	fluxapyroxad (BAS 700 F)
1309-64-4	antimony tri oxide
52-68-6	dimethyl 2,2,2-trichloro-1-hydroxyethylphosphonate; trichlorfon; DEP
7782-49-2	selemium
10108-64-2	chloride cadmium
1306-19-0	cadmium oxide
1163-19-5	decabromodiphenylether
1336-36-3	polychlorinated biphenyls
50008-00-3	tributyltin compounds (tributyltin oxide)
87-86-5	pentachlorophenol
	inorganic mercury

N° CAS	Flow not included in USETox	Comments
100-00-5	p-nitrochlorobenzene	Included in Lime 2 for ecotoxicity
100-44-7	benzyl chloride	
106-47-8	p-chloroaniline	
107-02-8	acrolein	
107-13-1	acrylonitrile	
108-42-9	m-chloroaniline	
108-95-2	phenol	
115-29-7	6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepine 3-oxide; endosulfan	
117-81-7	bis(2-ethylhexyl) phthalate	
117-84-0	di-n-octyl phthalate	
118-79-6		
12122-67-7	zinc N,N'-ethylenebis(dithiocarbamate); zineb	
121-75-5	O,O-dimethyl S-1,2-bis(ethoxycarbonyl)ethyl phosphorodithioate; malathon; malathion	
122-34-9	simazine	
137-26-8	tiuram	
137-30-4	zinc bis(N,N'-dimethyldithiocarbamate); ziram	
1563-66-2	2,3-dihydro-2,2-dimethyl-7-benzo[b]furanyl N-methylcarbamate; carbofuran	
1582-09-8	α,α,α-trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine; trifluralin	
17804-35-2	methyl N-[1-(N-n-butylcarbamoyl)-1H-2-benzimidazolyl]carbamate; benomyl	
1897-45-6	tetrachloroisophthalonitrile; chlorothalonil; TPN	
1912-24-9	2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine; atrazine	
21725-46-2	2-(4-chloro-6-ethylamino-1,3,5-triazin-2-yl)amino-2-methylpropiononitrile; cyanazine	
26444-49-5		
298-04-4	O,O-diethyl S-2-(ethylthio)ethyl phosphorodithioate; ethylthiometon; disulfoton	
330-54-1	3-(3,4-dichlorophenyl)-1,1-dimethylurea; diuron; DCMU	
330-55-2	3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea; linuron	
470-90-6	2-chloro-1-(2,4-dichlorophenyl)vinyl diethyl phosphate; chlorfenvinphos; CVP	
50-00-0	formaldehyde	
51218-45-2	2-chloro-2'-ethyl-N-(2-methoxy-1-methylethyl)-6'-methylacetanilide; metolachlor	
52645-53-1	3-phenoxybenzyl 3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate; permethrin	
534-52-1	4,6-dinitro-o-cresol	
60-51-5	O,O-dimethyl S-(N-methylcarbamoyl)methyl phosphorodithioate; dimethoate	
62-73-7	dimethyl 2,2-dichlorovinyl phosphate; dichlorvos; DDVP	
63-25-2	1-naphthyl N-methylcarbamate; carbaryl; NAC	
7439-92-1	lead	
7440-38-2	arsenic	
7440-47-3	chromium (+6)	
79-94-7		
82-68-8	pentachloronitrobenzene; quintozene; PCNB	
84-74-2	di-n-butyl phthalate	
85-68-7	n-butyl benzyl phthalate	

Addendum B – Some findings linked with LCIA methods and software implementation

Conducted by Neena Chandramathy and SABIC's LCA Team

The impact category analysis has been done to compare the uniformity of LCA results across methodologies and LCA software. The study has been done as a supporting document for the *Life Cycle Metrics for Chemical Products: A guideline by the chemical sector to assess and report on the environmental footprint of products.*

Scope: The impact category analysis has been done for the following ecoinvent data set for three methodologies; **ReCiPe Midpoint (H) V1.07, ILCD 2011 midpoint V1.01 and CML 2001**. The results have been included for the impact categories and intermediate flows as per the chemical sector guidelines. The two LCA software packages being used for the study are Simapro 7.3.3 and GaBi 6.

Data sets: The results are based on analysis of the five following data sets from ecoinvent database (v 2.2):

- 1 kg aluminium, primary, at plant/RER U;
- 1 kg nylon 6, at plant/RER U;
- 1 kg polyphenylene sulphide, at plant/GLO U;
- 1 kg injection moulding/RER U;
- 1 kg sheet rolling, aluminium/RER U.

Summary of results

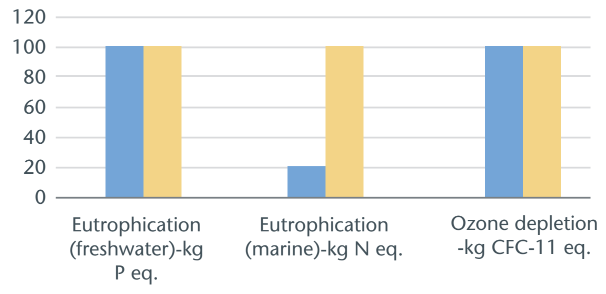
No.	Impact category	Unit	Meth1	Meth2	Meth3	Software	Key finding – methodology	Key finding – software
1	Photochemical ozone formation	kg C_2H_2 eq.			CML	Simapro and GaBi		Photochemical ozone formation has 17-70% variation by CML2011 (fig. ref. - 11- 15)
2	Resource depletion (fossil fuels)	kg Sb eq.		ILCD		Simapro and GaBi		Resource depletion (fossil fuels) has variation of ~ 2-43% by ILCD 2011 midpoint across software (fig. ref. - 11- 15)
3	Eutrophication (freshwater)	kg P eq.	ReCiPe	ILCD	CML	Simapro and GaBi	Eutrophication (freshwater)-kg P eq. has max. 50% (for nylon) variation in Simapro for ReCiPe and ILCD; but ~90% variation in GaBi (fig. ref. - 1- 10)	Eutrophication (freshwater) by ReCiPe Midpoint (H) V1.07 has 0-90% variation. ~0-50% variation by ILCD 2011 midpoint. 3-59% variation by CML 2011 (fig. ref. - 11- 15)
4	Eutrophication (marine)	kg N eq.	ReCiPe	ILCD		Simapro and GaBi	Eutrophication (marine)-kg N eq. has 58 - 79% variation in Simapro for ReCiPe and ILCD (fig. ref. - 1- 10)	Eutrophication (marine) has variation of ~ 65-100% by ReCiPe Midpoint (H) V1.07 across software (fig. ref. - 11-15)
5	Human toxicity (cancer effects)	CTUh		ILCD		Simapro and GaBi		Human toxicity (cancer effects) has very low variation across software. (fig. ref.- 11- 15)
6	Human toxicity (non-cancer effects)	CTUh		ILCD		Simapro and GaBi		Human toxicity (non-cancer effects) has variation of ~ 49-81% by ILCD 2011 midpoint across software (fig. ref. - 11-15)
7	Ecotoxicity	CTUe		ILCD		Simapro and GaBi		Eco-toxicity has variation of ~ 4-87% by ILCD 2011 midpoint across software (fig. ref. - 11- 15)
8	Dust and particulate matter	kg PM2.5 eq.		ILCD		Simapro and GaBi		Dust and particulate matter has variation of ~8-46% by ILCD 2011 midpoint across software (fig. ref. - 11- 15)
9	Ozone depletion	kg CFC-11 eq.	ReCiPe	ILCD	CML	Simapro and GaBi	Ozone depletion - kg CFC-11 eq. has 2-13% variation in Simapro for ReCiPe and ILCD; 10 -22% variation in GaBi)	Ozone depletion by ReCiPe Midpoint (H) V1.07 is consistent across software. ~3-23% variation by ILCD 2011 midpoint. 4-35% variation by CML 2011. (fig. ref. - 11- 15)
10	Land occupation	m2a	ReCiPe			Simapro and GaBi		Land occupation by ReCiPe Midpoint (H) V1.07 is consistent across software

Table 1: Summary of results

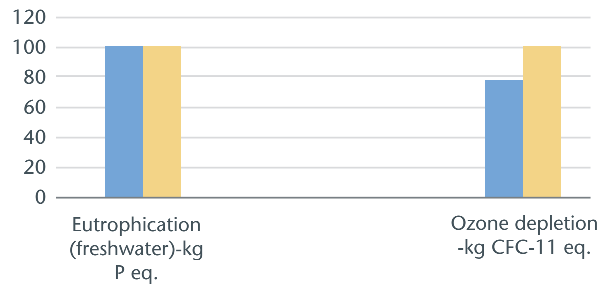
Detailed results - comparison of impact categories across methodology

🟦 Recipe Midpoint (H) v1.07 🟨 ILCD 2011 Midpoint

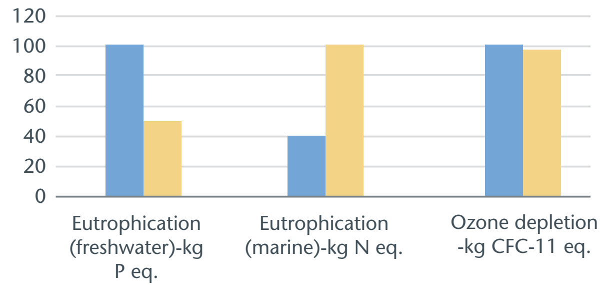
1 kg aluminium, primary, at plant/RER U-Simapro 7.3.3



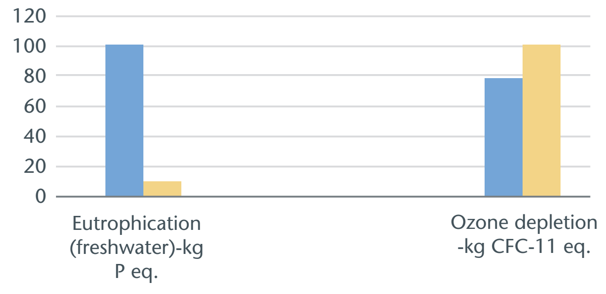
1 kg aluminium, primary, at plant/RER U-GaBi 6



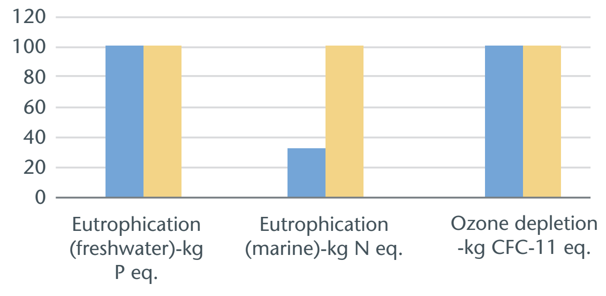
1 kg nylon 6, at plant/RER U-Simapro 7.3.3



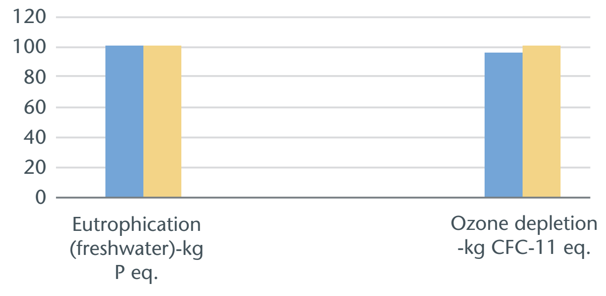
1 kg nylon 6, at plant/RER U-GaBi 6



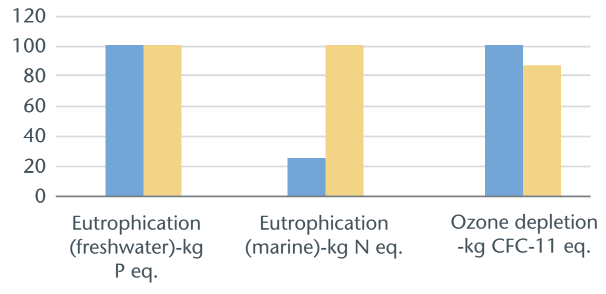
1 kg polyphenylene sulfide, at plant/GLO U-Simapro 7.3.3



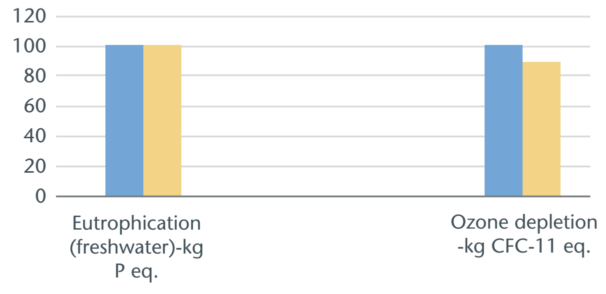
1 kg polyphenylene sulfide, at plant/GLO U-GaBi 6



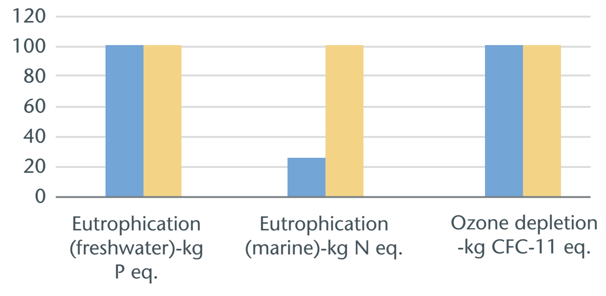
1 kg injection moulding/RER U-Simapro 7.3.3



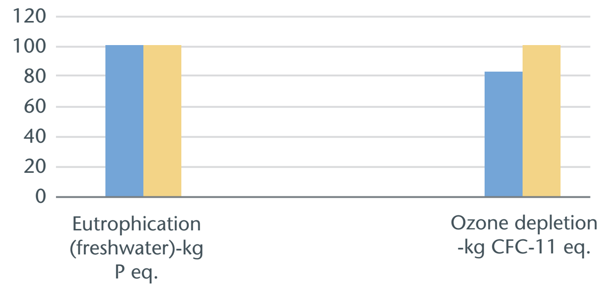
1 kg injection moulding/RER U-GaBi 6



1 kg sheet rolling, aluminum/RER U-Simapro 7.3.3



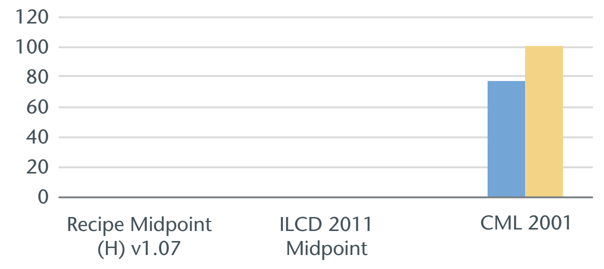
1 kg sheet rolling, aluminum/RER U-GaBi 6

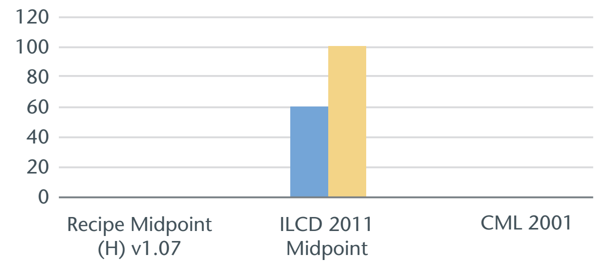


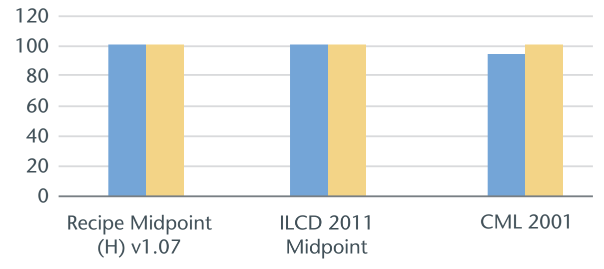
Detailed results - comparison of impact categories across software

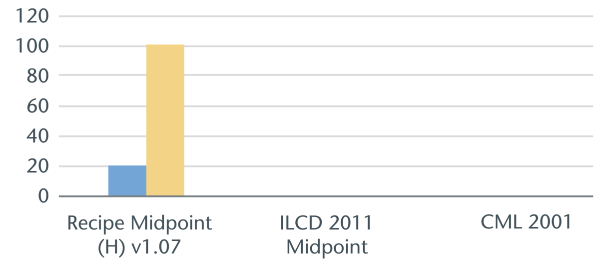
1 kg aluminium, primary, at plant/RER U

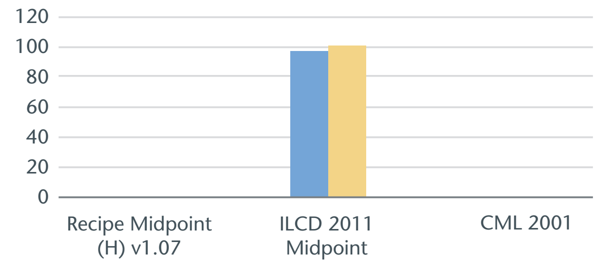
🟦 Simapro 7.3.3 🟨 GaBi 6

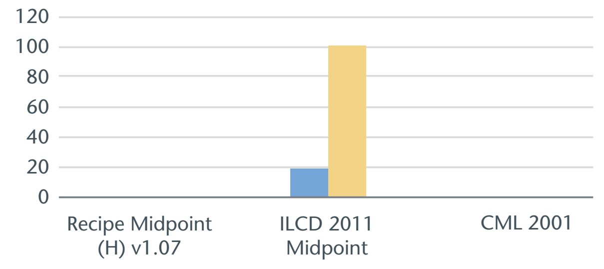

Photochemical ozone formation-kg C2H2 eq.

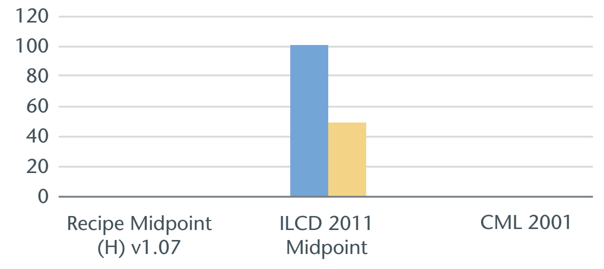

Resource depletion (fossil fuels)-kg Sb eq.

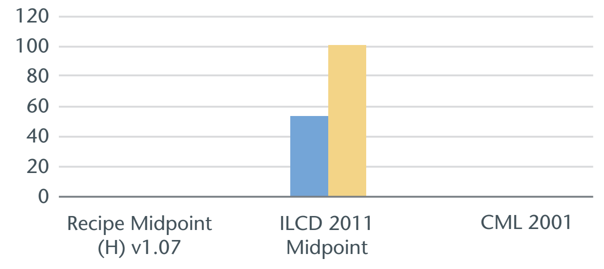

Eutrophication (freshwater)-kg P eq.

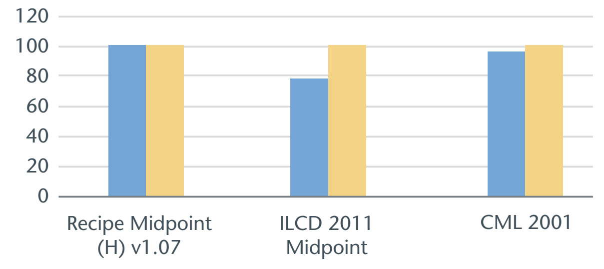

Eutrophication (marine)-kg N eq.

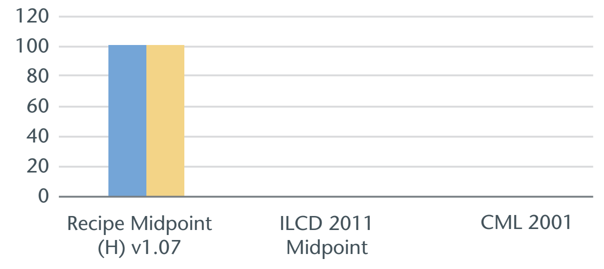

Human toxicity (cancer effects)-CTUh


Human toxicity (non-cancer effects)-CTUh


Ecotoxicity – CTUe


Dust and particulate matter-kg PM2,5 eq.

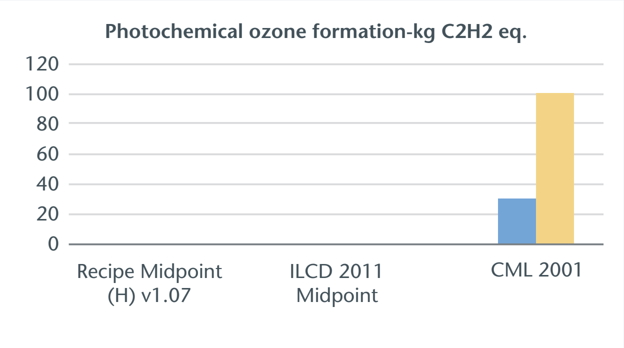

Ozone depletion-kg CFC-11 eq.

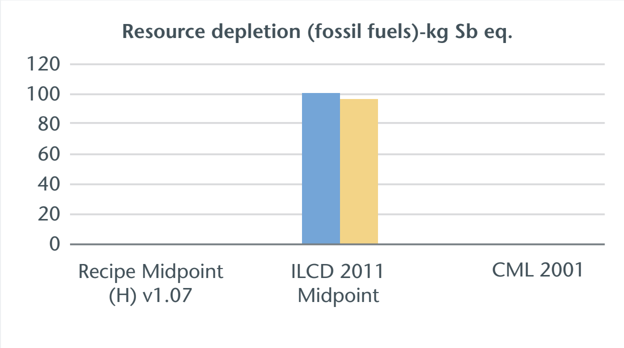

Land occupation-m²a

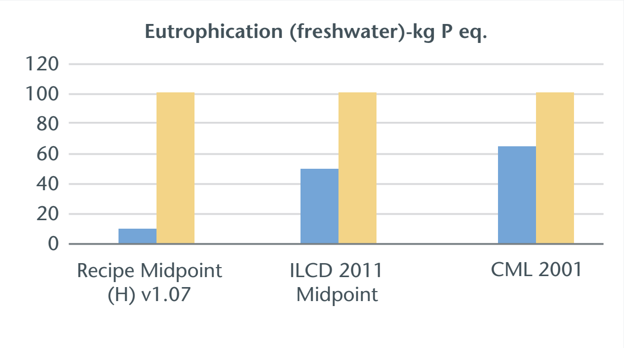
Detailed results - comparison of impact categories across software

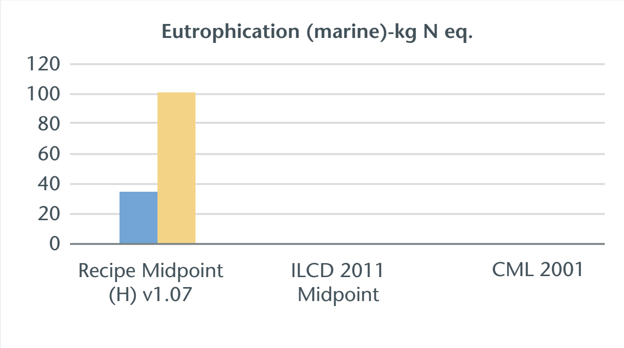
1 kg nylon 6, at plant/RER U

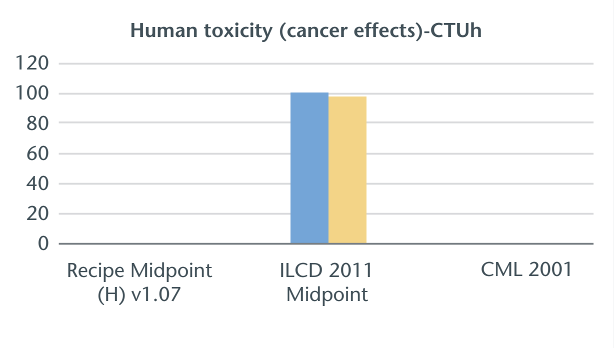
🟦 Simapro 7.3.3　🟨 GaBi 6

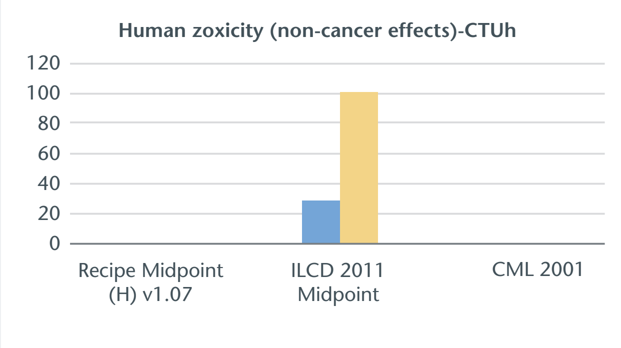

Photochemical ozone formation-kg C2H2 eq.

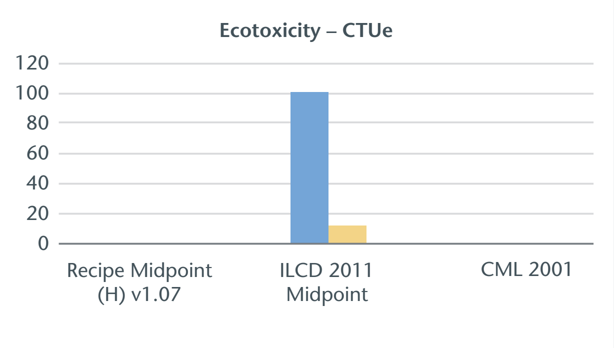

Resource depletion (fossil fuels)-kg Sb eq.

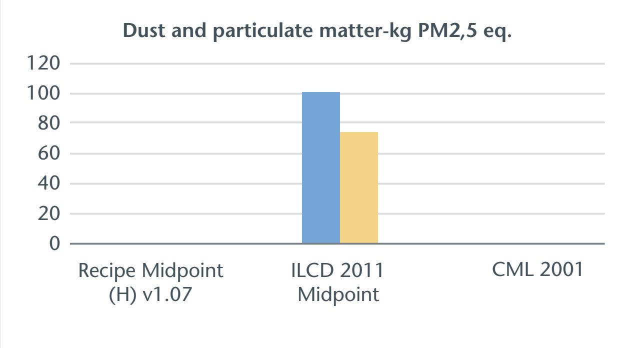

Eutrophication (freshwater)-kg P eq.

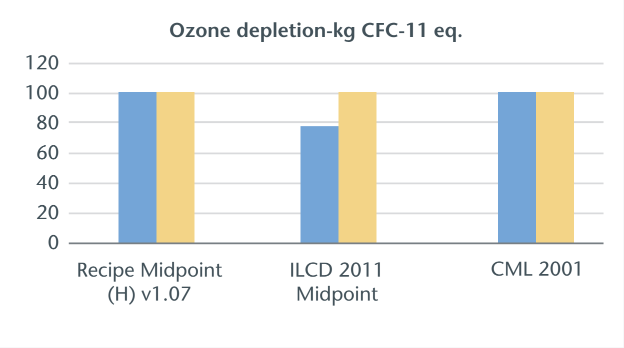

Eutrophication (marine)-kg N eq.

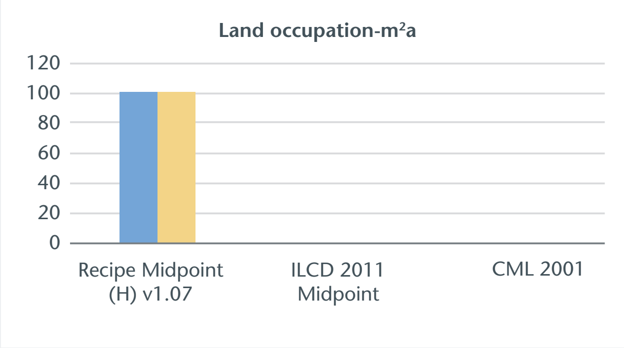

Human toxicity (cancer effects)-CTUh


Human zoxicity (non-cancer effects)-CTUh


Ecotoxicity – CTUe


Dust and particulate matter-kg PM2,5 eq.

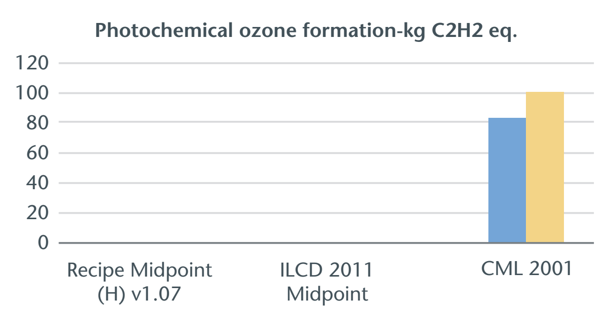

Ozone depletion-kg CFC-11 eq.

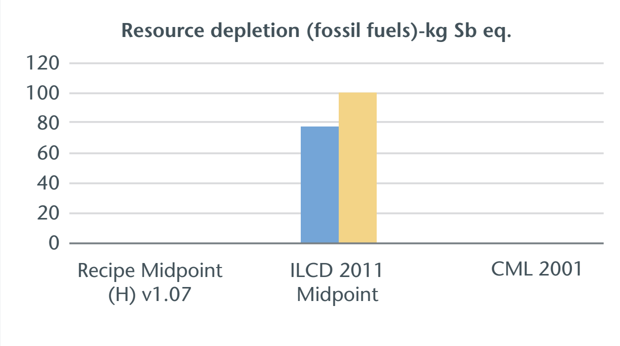

Land occupation-m^{2}a

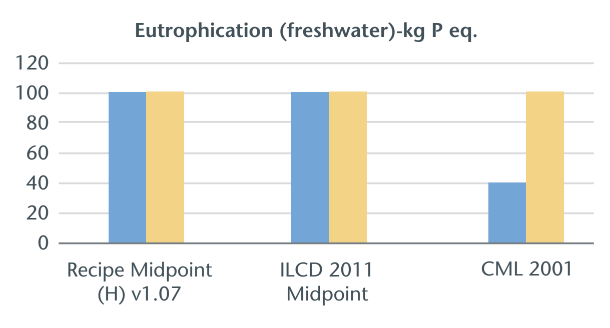
Detailed results - comparison of impact categories across software

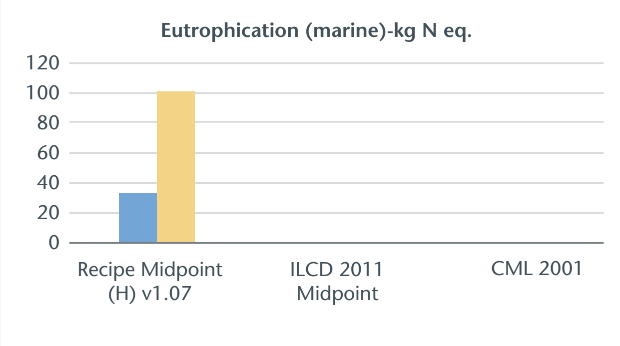
1 kg polyphenylene sulfide, at plant/GLO U

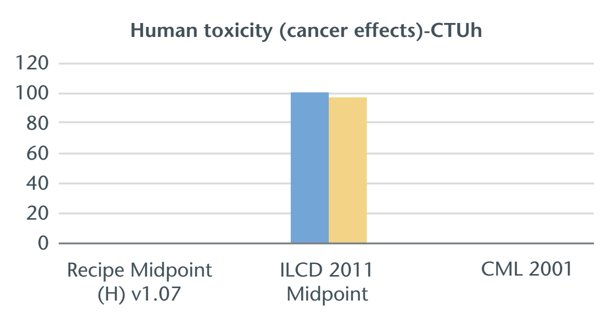
🟦 Simapro 7.3.3 🟨 GaBi 6

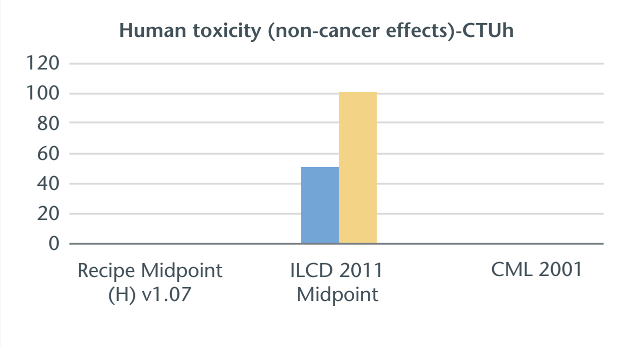


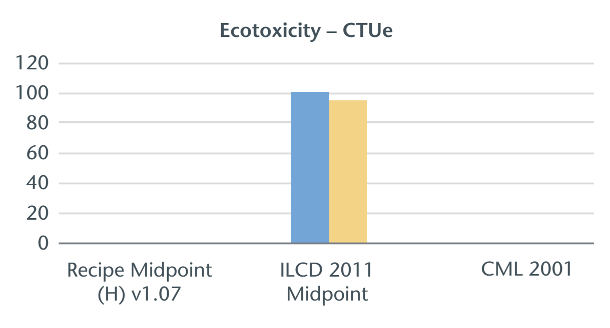


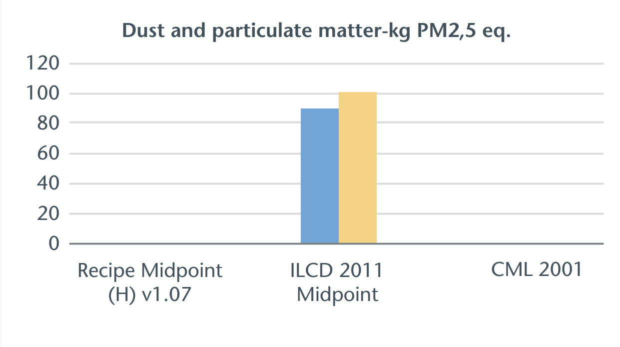


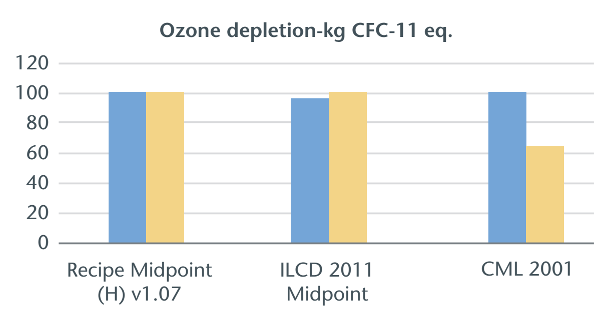


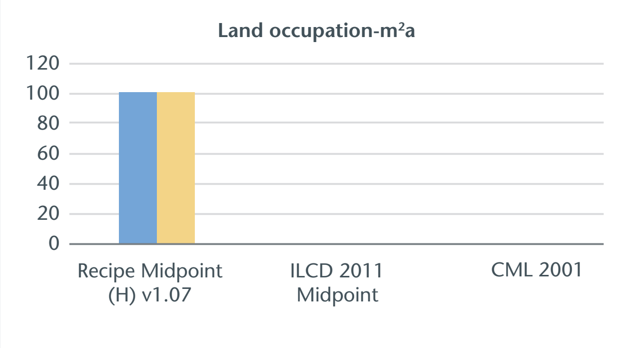












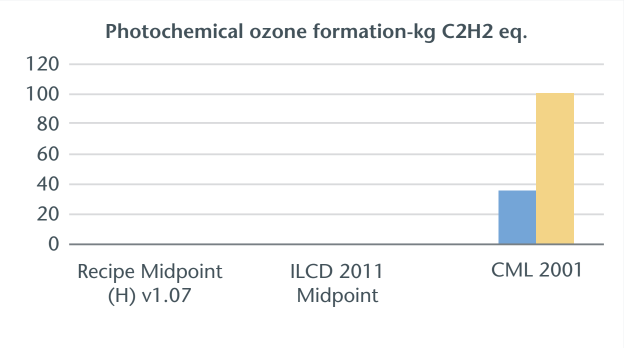
Detailed results - comparison of impact categories across software

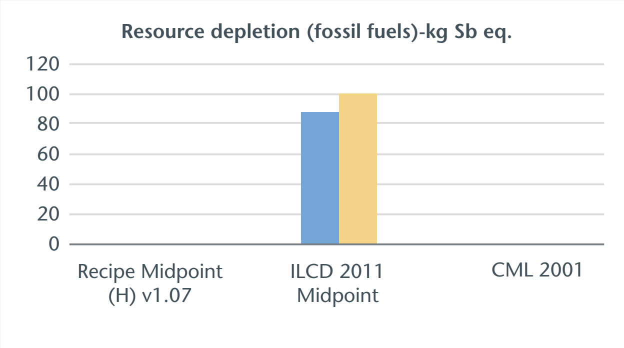
1 kg injection moulding/RER U

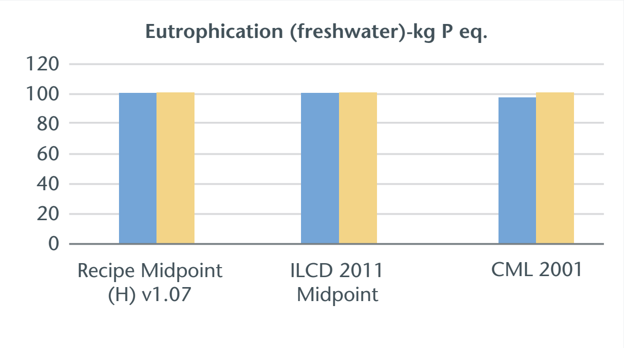
Detailed results - comparison of impact categories across software

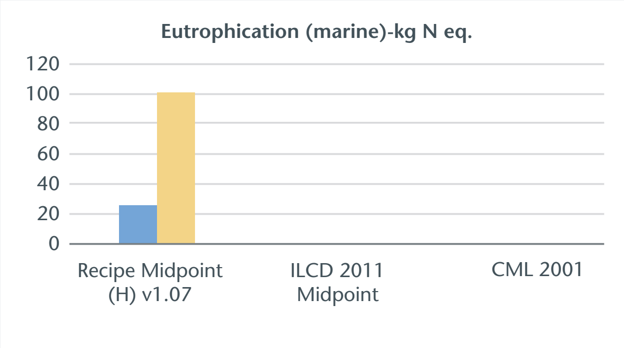
1 kg sheet rolling, aluminum/RER U

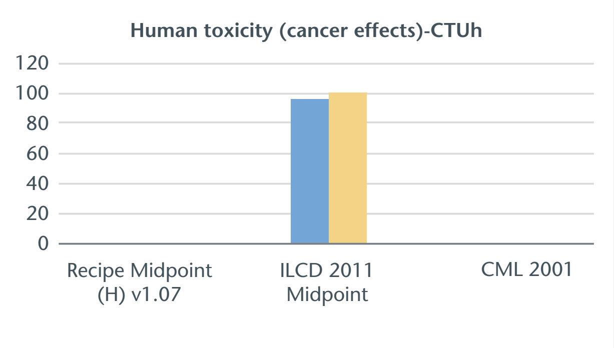
🟦 Simapro 7.3.3 🟨 GaBi 6

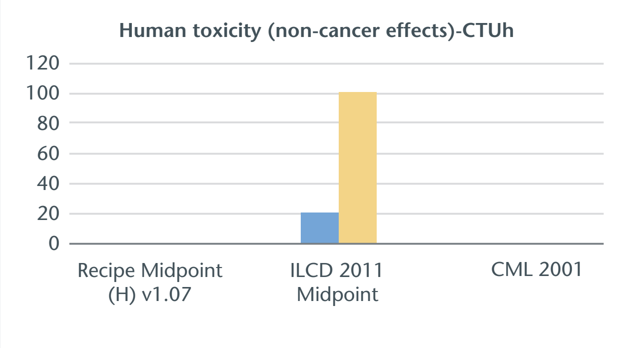

Photochemical ozone formation-kg C2H2 eq.

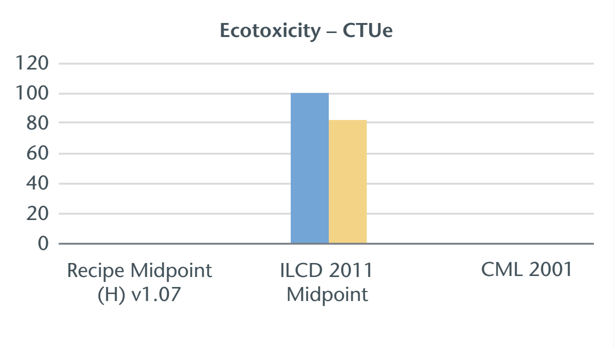

Resource depletion (fossil fuels)-kg Sb eq.

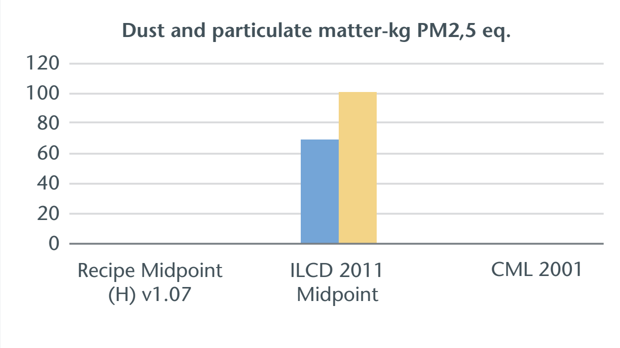

Eutrophication (freshwater)-kg P eq.

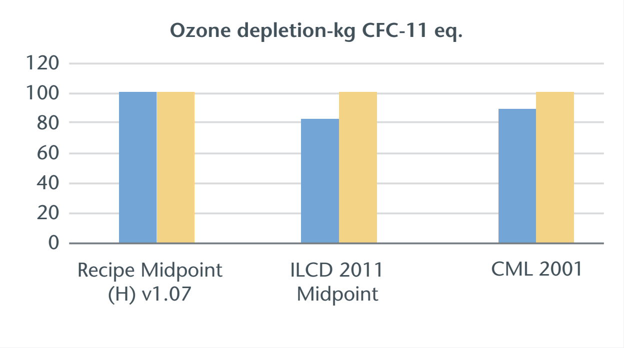

Eutrophication (marine)-kg N eq.

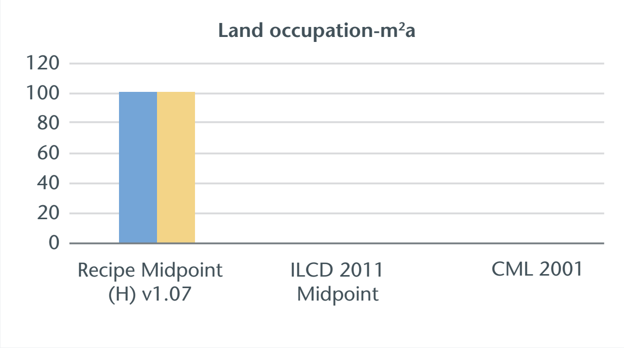

Human toxicity (cancer effects)-CTUh


Human toxicity (non-cancer effects)-CTUh


Ecotoxicity – CTUe


Dust and particulate matter-kg PM2,5 eq.


Ozone depletion-kg CFC-11 eq.


Land occupation-m^{2}a

Addendum C – Some findings linked the comparison of human toxicity and eco-toxicity impact assessment methods

Conducted by Jean François Viot and Solvay's LCA Team

Comparative analysis of processes with a series of impact characterisation methods

Data sets

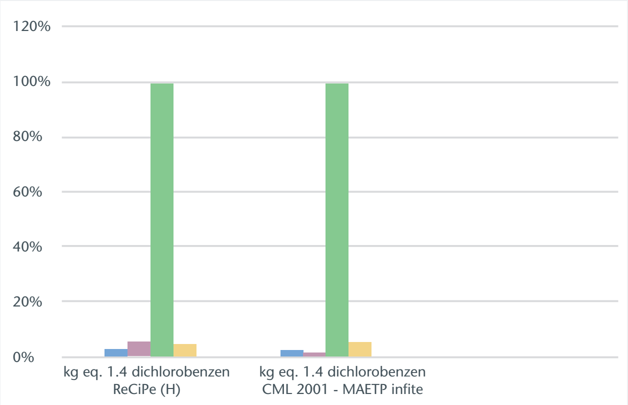
The results are based on analysis of the five following data set from ecoinvent database (v 2.2):

- 1 MJ of heat, at hard coal industrial furnace 1-10 MW/RER;
- 1 kg sodium hydroxide, 50 percent in H_2O, production mix, at plant/RER;
- 1 kg palm fruit bunches, at farm/MY;
- 1 kg toluene, liquid, at plant/RER.

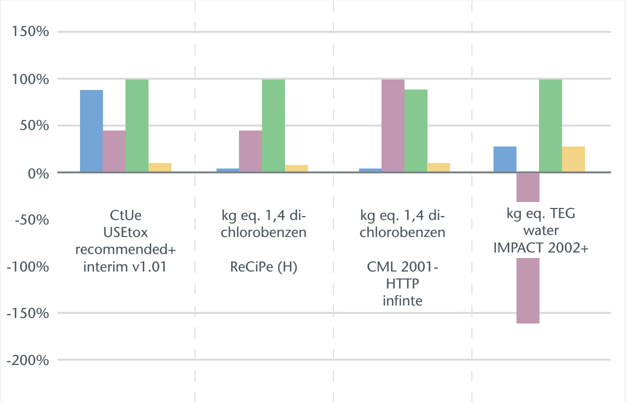
Summary of results

- Depending on the characterization method, the relative position of the different processes are not the same.
- Negative values appear for "palm fruits" due to the inventory of trace elements (Zn and Cu) during cultivation (*Nemecek model for trace elements).*

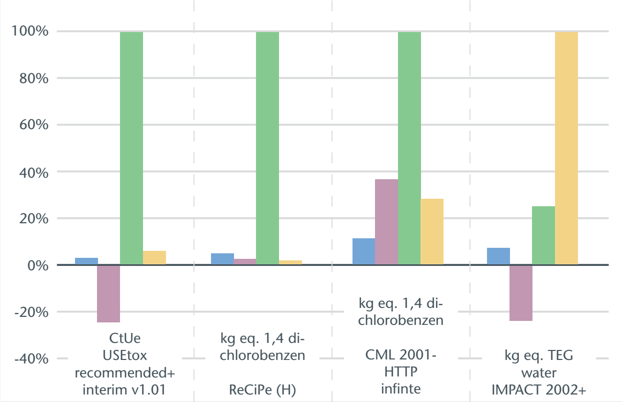
Ecotoxicity marine
% of the highest impact for each method



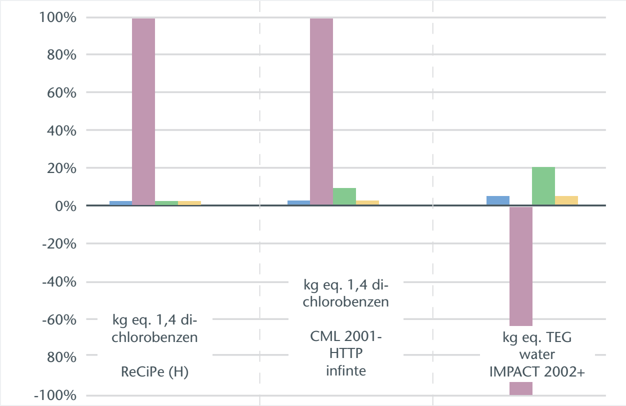
Ecotoxicity fresh water
% of the highest impact for each method

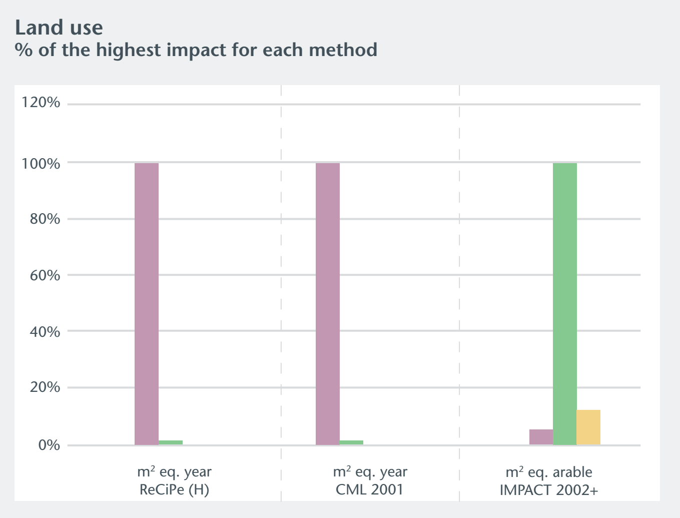


Human toxicity
% of the highest impact for each method



Ecotoxicity terrestrial
% of the highest impact for each method





Land use
% of the highest impact for each method

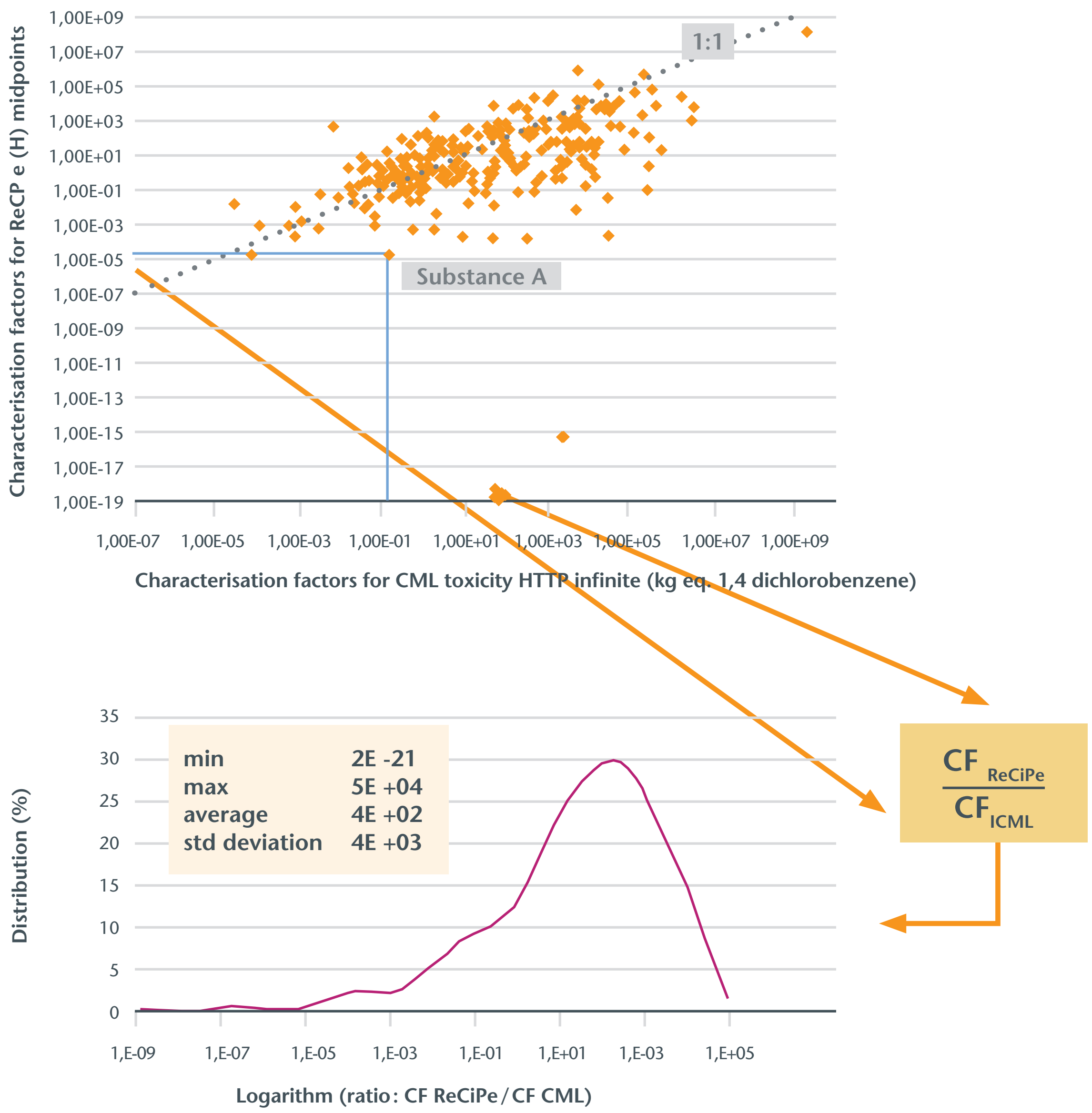
Most contributing substances in analysed impacts, according to the different methods

The table below shows high discrepancies due to (based on ongoing analysis): i) update of characterisation factors, ii) completeness of substances / compartments and iii) modelled impacts.

		Heat from coal	Palm fruit bunches	Sodium hydroxyde	Toluene
Human toxicity	CML 2001	**Chromium VI** Air – high population	**Benzene** Air – low population	**Selenium** Water – groundwater, long-term	**Nickel** Air – high population
	USEtox	**Antimony** Water – groundwater, long-term	**Zinc** Soil – agricultural	**Mercury** Air – high population	**Chromium VI** Water – groundwater, long-term
	IMPACT 2002+	**Arsenic, ion** Water – River	**Zinc** Soil – agricultural	**Arsenic, ion** Water – river	**Hydrocarbons, aromatic** Air – high population
	ReCiPe (H)	**Manganese** Water – groundwater, long-term	**Arsenic** Air – low population, long-term	**Manganese** Water – groundwater, long-term	**Antimony** Water – groundwater, long-term
Ecotoxicity, freshwater	CML 2001	**Nickel, ion** Water – groundwater, long-term	**Cypermethrin** Soil – agricultural	**Nickel, ion** Water – groundwater, long-term	**Copper, ion** Water – groundwater, long-term
	USEtox	**Chromium VI** Water – groundwater, long-term	**Carbofuran** Soil – agricultural	**Chromium VI** Water – groundwater, long-term	**Antimony** Water – groundwater, long-term
	IMPACT 2002+	**Aluminium** Air – unspecified	**Copper** Soil – agricultural	**Aluminium** Water – river	**Aluminium** Water – river
	ReCiPe (H)	**Nickel, ion** Water – groundwater, long-term	**Cypermethrin** Soil – agricultural	**Nickel, ion** Water – groundwater, long-term	**Nickel, ion** Water – groundwater, long-term
Ecotoxicity, marine	CML 2001	**Beryllium** Water – groundwater, long-term	**Beryllium** Water – groundwater, long-term	**Beryllium** Water – groundwater, long-term	**Nickel** Air – high population
	ReCiPe (H)	**Nickel, ion** Water – groundwater, long-term	**Cypermethrin** Soil – agricultural	**Nickel, ion** Water – groundwater, long-term	**Nickel** Air – high population
Ecotoxicity, terrestrial	CML 2001	**Mercury** Air – high population	**Cypermethrin** Soil – agricultural	**Mercury** Air – high population	**Nickel** Air – high population
	IMPACT 2002+	**Aluminium** Air – unspecified	**Copper** Soil – agricultural	**Aluminium** Soil – agricultural	**Nickel** Air – high population
	ReCiPe (H)	**Copper** Air – high population	**Cypermethrin** Soil – agricultural	**Mercury** Air – high population	**Nickel** Air – high population
Land use	CML 2001	**Occupation – dump site**	**Occupation – forest, intensive, short cycle**	**Occupation – forest, intensive, normal**	**Occupation – dump site**
	IMPACT 2002+	**Occupation – industrial area**	**Occupation – forest, intensive, normal**	**Occupation – forest, intensive, normal**	**Occupation – forest, intensive, normal**
	ReCiPe (H)	**Occupation – dump site**	**Occupation – forest, intensive, short cycle**	**Occupation – forest, intensive, normal**	**Occupation – dump site**

Table 2: Discrepancies

Comparison of characterization factors between CML Human Toxicity and ReCipE for the same substances



Comparison of characterisation factors between CML Human Toxicity and ReCipE for the same substances

12. Case studies

Case study one

The environmental effects of type 4 compressed natural gas tanks with Akulon fuel lock liners for transport applications

Commissioner: T. Vorage, Application Development Manager, DSM Engineering Plastics

LCA Practitioner: H. Bosch, LCA Competence Leader, DSM Corporate Operations and Responsible Care

Date: December 18, 2013

In-depth comparative analysis of characterisation factors: example of human toxicity - CML vs ReCiPe (H)

- 1,846 substances[13] are taken into account by either CML or ReCiPe, of which:
  - 885 are taken into account by CML;
  - 1,209 are taken into account by ReCiPe;
  - **248 are taken into account by both;**
  - 1,598 are taken into account by only one of the two methods.
- Both CML and ReCiPe characterisation factors for human toxicity are based on the effect on human health of emitted substances, potentially in contact with humans by either inhalation or ingestion.
- They are expressed in the same unit (same reference substance: 1,4 DCB).
- Fate factors, exposure factors and effect factors are based on different and **complex** models.
- ReCiPe is more documented.

This study was conducted according to the requirements of the WBCSD *Life Cycle Metrics for Chemical Products: A guideline by the chemical sector to assess and report on the environmental footprint of products* and according to the ISO 14040:2006 and 14044:2006 standards.

The detailed methodological report can be obtained from the commissioner.

1. Scoping

1.1. Goal and scope definition

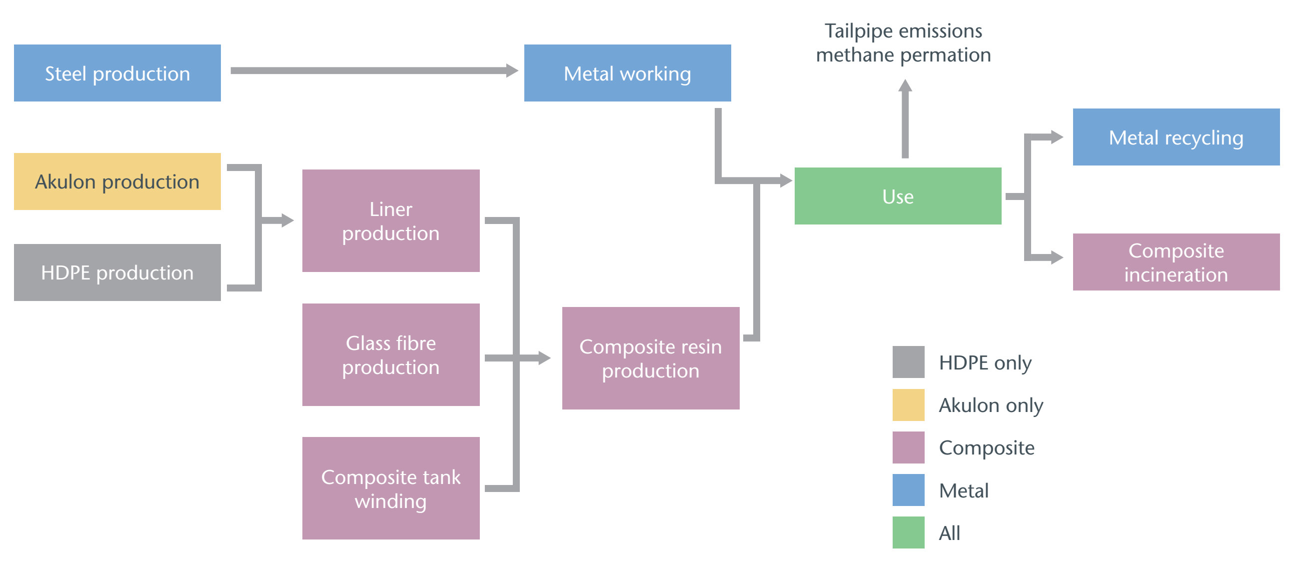
1.1.1. Intended application(s) of the study

The intended application of this chemical product footprint study is to explain the environmental effects of using Akulon fuel lock lined type 4 compressed natural gas tanks compared to metal or high-density polyethylene (HDPE) lined tanks.

1.1.2. Reasons for carrying out the study

The reason to carry out this study is to provide compelling evidence to potential customers that the Akulon fuel lock lined tanks are environmentally superior to competing solutions.

Figure 1: Processes included in this study



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[13] substance/compartment/subcompartment

1.1.3. Business goal

The business goal of this study is to increase sales by providing potential customers with more convincing information about the environmental benefits of composite compressed natural gas tanks.

1.1.4. Target audience

The target audience is potential customers but also other parties further downstream in the value chain.

1.2. System boundaries

1.2.1 System boundaries description

All steps in the product life cycle are included for the manufacturing of the tanks – from extraction of materials from the earth, through various processing steps, until the complete tank. Emissions associated with the production and combustion of gasoline to transport the fuel tanks in the use phase are included, as well as the methane emissions permeating through the composite tank liners. Finally, disposal and/or recycling at the end-of-life are included.

For all background processes, it is assumed they occur in Europe, following the ecoinvent policy on Union for the Coordination of the Transmission of Electricity (UCTE) electricity use.

1.2.2. Limitation statement

For the use phase, only the emissions attributable to the transport of the tanks are included. Other impacts related to the vehicle are independent of the type of tank used and therefore excluded from the scope.

It is assumed that the tanks do not require any finishing steps, such as coating. The metal tank might need a coating, but the effect of coating is assumed to be very small when compared to other contributors, and including it would only increase the impact of the metal tank, reinforcing the conclusions of this study.

It is assumed that all tanks outlive the vehicle they are built into, require no maintenance, and cannot be reused in another vehicle. Therefore, tank maintenance and reuse are excluded from the scope.

1.3. Functional unit

1.3.1. Function description

Providing compressed natural gas storage capacity for one car during the complete lifetime

1.3.2. Functional unit description

1. One compressed natural gas tank

1.3.3. Comparability statement

All alternative tanks are designed to require no maintenance and to outlive the vehicle. There is very little need for replacement tanks and after life, as tanks are not reused. Therefore, the benefit for the compared solutions is the same in all cases: providing natural gas storage capacity for one car during the complete lifetime.

The tanks compared are completely interchangeable. This is guaranteed by verified legal requirements for product approval. There are no differences in technical quality that affect the life cycle of the alternatives.

None of the tanks provide any additional functions that should be accounted for.

The systems modelled and compared are fully equivalent in the use phase. All tanks are designed to contain the same amount of compressed natural gas at the same maximum pressure.

1.3.4. Service life

The average service life of a car is assumed to be 10 years. The maximum service life is much longer and does not impose any practical limits.

1.3.5. Duration of the functional unit

This is not relevant for cradle-to-grave studies like this one.

2. Methodological choices

2.1. Choices for impacts and flows

The impacts presented in this study are in accordance with the *Life Cycle Metrics for Chemical Products* guideline, as far as these are available in SimaPro. If the preferred option is not available in SimaPro, those methods with the best similarity are used. This means this report is not compliant with the guideline in this respect.

Impact category	Guideline choice		Our choice		Agreement with WBCSD
	Indicator	Characterisation model	Indicator	Method	
Global warming	kg CO_2 eq.	Global warming potential infrared radiative forcing (100 year)	kg CO_2 eq.	ILCD	Yes
Photochemical ozone formation	kg Ethylene eq.	LOTOS-EUROS	kg Ethylene eq.	ILCD	Yes, unit is converted
Air acidification	mol H+ eq.	Accumulated Exceedance model	mol H+ eq.	ILCD	Yes
Resource depletion (fossil fuels)	MJ	CML 2002 model	kg Sb eq.	ILCD	Yes, but different unit
Abiotic depletion (element)	kg Sb eq.	CML 2002 model	kg Sb eq.	ILCD	Yes
Eutrophication (freshwater)	kg P eq.	EUTREND model	kg P eq.	ILCD	Yes
Eutrophication (marine)	kg N eq.	EUTREND model	kg N eq.	ILCD	Yes
Human toxicity – cancer	CTUh	USETox Model	CTUh	ILCD	Yes
Human toxicity – non-cancer	CTUh	USETox Model	CTUh	ILCD	Yes
Ecotoxicity	CTUh	USETox Model	CTUe	ILCD	Yes
Dust & particulate matter	kg PM2.5 eq.	Riskpoll model	kg PM2.5 eq.	ILCD	Yes
Land use	kg C*yr	Model based on Soil Organic Matter (SOM)	m^2a	ILCD	Yes
Species richness	m^2*yr	ReCiPe (endpoint) or Koellner	species.yr	ReCiPe (Europe H/A endpoint)	Yes
Ozone Depletion	kg CFC-11 eq	World Meteorological Organization over an infinite time horizon, as implemented in EDIP	kg CFC11 eq	EDIP	Yes
Water depletion	m^3	Swiss Ecoscarcity model	m^3	ILCD	Yes

Table 1: Choices for impact and flows

The photochemical ozone formation results were converted from non-methane-volatile organic compounds (NMVOC) equivalents to ethylene equivalents by dividing by the characterisation factor of ethylene in the model (1.69 kg NMVOC-eq/kg ethylene).

For fossil fuel depletion, there is a discrepancy between the literature source and the indicator unit in the chemical products guideline. The method referred to measures in kg Sb equivalents and not in MJ. In addition, the ILCD method does not include an indicator for fossil fuel separately. The reported values are the subset of the element abiotic depletion method in the *ICLD Handbook* related to fossil fuel only.

The energy-related flows required by the WBCSD guideline are also presented:

- Cumulative energy demand (in MJ);
- Renewable energy consumption (in MJ);
- Non-renewable energy consumption (in MJ).

Impact categories and flows that are not mandatory to report according to the guideline are not reported in this report.

2.2. Allocation rules between co-products

There are no significant co-products in the downstream parts of the value chain. For upstream processes, ecoinvent models and the associated allocations were used. The greatest occurrence of allocation is in refineries and crackers for the production of organic basic building blocks used in the type 4 tanks. The ecoinvent method of allocation is widely accepted.

2.3. Attribution of recycling benefits

It is assumed that all steel is recycled at the end of its life. Steel recycling is taken into account in accordance with guidelines of the steel industry by using ecoinvent models for primary and secondary steel, with only make-up primary steel to compensate yield losses in secondary steel making.

2.4. Avoided emissions

Avoided emissions are not relevant in this study.

2.5. Biogenic uptake and emissions

Biogenic uptake or emissions are not relevant in this study.

2.6. Carbon storage and delayed emissions

Carbon storage and delayed emissions are not relevant in this study.

2.7. Direct land-use change / indirect land-use change

Land-use change effects are not relevant in this study.

3. Data sources

3.1. Life cycle inventory analysis procedures

Data was supplied by the commissioner, T. Vorage. He collected them from reliable sources, such as DSM measurements and design data.

3.2. Data sources description

Table 2 lists the sources of the data used.

Life cycle stage	Item	Category	Origin/source type
Extraction	All	Secondary	ecoinvent
Materials production	Steel	Secondary	ecoinvent
	Glass fibre	Secondary	Glass Fibre Europe
	Epoxy resin	Secondary	ecoinvent
	Akulon fuel lock	Primary	DSM
	HDPE	Secondary	ecoinvent
Tank manufacture	Type 4 tanks	Secondary	ecoinvent and DSM estimates of intensities
	Steel tank	Secondary	ecoinvent and DSM estimates of intensities
Use	Fuel consumption	Secondary	Automotive industry estimate[2]
	Fuel emissions	Secondary	ecoinvent
	Methane emissions	Primary	Measured in DSM lab
End-of-life	Steel tanks	NA	Zero impact assuming steel is recycled
	Incineration of type 4 tanks	Secondary	ecoinvent

Table 2: Data sources used

3.3. Data used

The values of the key parameters used in this study are listed in the table 3 below.

Parameter	Unit	Value
Weight of steel tank	kg	32
Weight of glass fibre in composite tank	kg	12
Weight of resin in composite tank	kg	3
Weight of aluminum bosses of composite tank	kg	0.6
Weight of HDPE liner	kg	4.3
Weight of Akulon® fuel lock liner	kg	2.2
Car life time	years	10
Annual driver distance	km	23000
Fuel reduction value	l/100 kg/100 km	0.34
Average tank pressure	bar	105
Methane permeability HDPE	g mm / (m^2 year bar)	40
Methane permeability Akulon® fuel lock liner	g mm / (m^2 year bar)	0.24
Thickness HDPE liner	mm	3
Thikness Akulon® fuel lock liner	mm	1.5

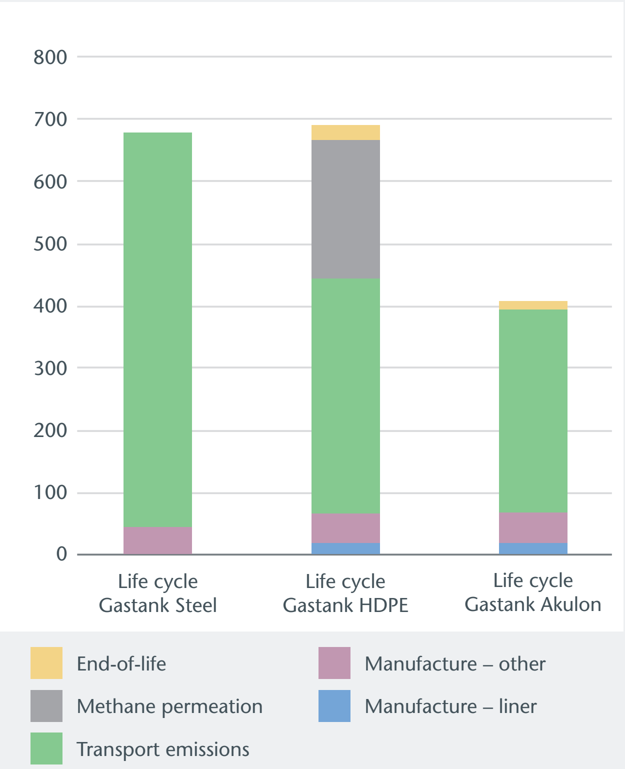
Table 3: Values of the key parameters used in this study

The fuel reduction value is reported in literature for petrol fueled cars. It has been converted to natural gas using the ratio of lower heating values of the two fuels.

4. Results and interpretation

The rationale for switching from steel tanks to composite tanks is that the reduced weight lowers the cars fuel consumption, and thereby the tailpipe emissions, primarily CO_2 and other greenhouse gases. In composite tanks with an HDPE liner, this reduction is compensated by emissions of methane permeated through the tank. The figure below shows the breakdown of the carbon footprint of the three tanks.

Figure 2: Carbon footprint breakdown



In all three cases, the emissions caused by the combustion of fuel to transport the tank are dominant. This is why the weight reduction effectively reduces the carbon footprint. The impacts of manufacturing the tanks are very similar because the higher impact per kg of material for the composite tanks offsets the lighter weight materials. The contribution of the impact of manufacturing the liner is very limited. They are very similar for the two cases, because the lighter weight Akulon fuel lock liner is offsets by a higher impact per kg. The contribution of end-of-life emissions for the composite tanks is also limited. For the HDPE tank, the benefit of weight reduction is offset by the effect of methane emissions.

Overall results for all impact categories are given in table 4.

Impact category	Indicator	Steel	HDPE	Akulon
Global warming	kg CO_2 eq	687	699	412
Photochemical Ozone Formation	kg Ethylene eq	1.23	0.94	0.80
Air acidification	molc H+ eq	1.90	1.33	1.21
Resource Depletion (fossil fuels)	g Sb eq	0.08	0.05	0.05
Abiotic Depletion (element)	g Sb eq	2.4	1.0	1.0
Eutrophication (freshwater)	g P eq	54	28	25
Eutrophication (marine)	g N eq	87	60	54
Human Toxicity Cancer	µCTUh	0.25	0.48	0.47
Human Toxicity Non-Cancer	µCTUh	0.04	0.15	0.14
Ecotoxicity	CTUe	1.7	2.6	8.8
Dust & Particulate Matter	kg PM2.5 eq	0.13	0.11	0.10
Land use	kg C deficit	16	35	34
Species richness	µspecies.yr	5.4	5.6	3.3
Ozone Depletion	mg CFC11 eq	92	55	50
Water scarcity	m^3 eq	0.30	0.36	0.36

Table 4: Overall results by impact categories

In most environmental impact categories, the composite tanks have a lower impact than the steel tank. This is related to the lighter composite tanks, reducing fuel consumption and emissions during the use phase. In most cases, the Akulon fuel lock impacts are slightly lower than the HDPE impacts because the Akulon fuel lock liner is lighter than the HDPE liner.

The global warming effect of the methane permeation in the HDPE case also affects species richness, which is dominated by climate change.

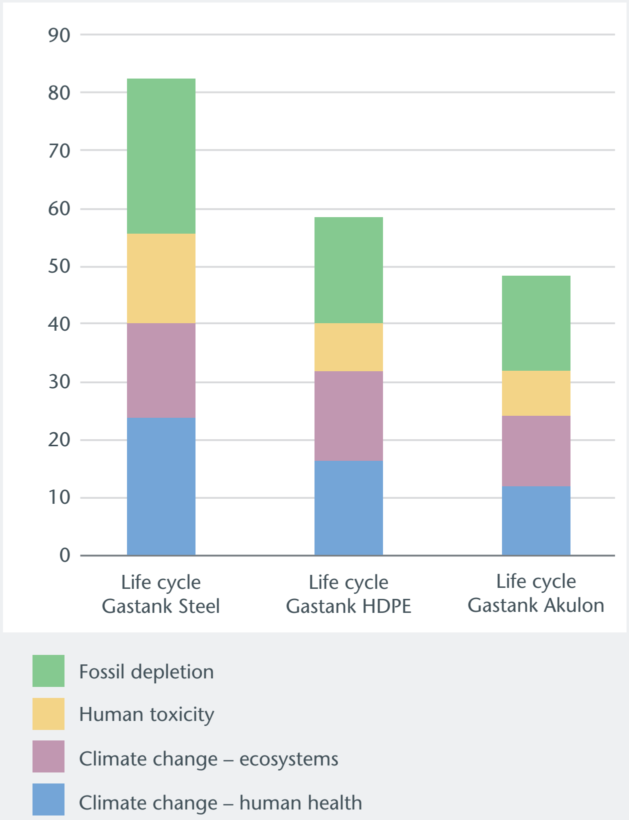
The toxicity impacts are much higher for the composite tanks due to specific upstream emissions, such as nitrobenzene to water, and of styrene to air in the winding operation. The ecotoxicity effect of the Akulon fuel lock tank is much higher due to the emission of cumene to water upstream in the PA 6 production process.

The land-use impacts of the two composite containers are both higher than the impact of the steel tank. This is due to the harvesting of timber to produce packaging cardboard for the blow-moulded liners. This process contributes very little to other impacts, but because there is so little land use in other processes, it dominates the land-use impacts.

Water scarcity impact are higher for the composite tanks, however we consider the overall water consumption low compared to other value chains, and the inventories used are not very reliable regarding water consumption.

The composite tanks perform better in almost all categories, and Akulon fuel lock scores slightly better than HDPE, and much better for climate change and species richness. The only exceptions are water scarcity, land use and, more extremely, toxicity. The question is if these impacts should be weighed heavily in the selection of a tank design. To get an impression of the relative importance of toxicity, a method is needed that weights the impacts in various categories. Results for the ReCiPe E/A method are shown in the figure below. According to the developers, this version of ReCiPe deals with toxicity impact in a way similar to USEtox, and it gives them the highest weight in relative terms.

Figure 3: Environmental impacts according to ReCiPe E/A Europe



Considering their lower contribution to the total aggregated impact, the following impact categories are not visible on the graph: Metal depletion, natural land transformation, urban land occupation, agricultural land occupation, Ionising radiation, marine ecotoxicity, freshwater ecotoxicity, terrestrial ecotoxicity, particulate matter formation, photochemical oxidant formation, freshwater eutrophication, terrestrial acidification, ozone depletion.

With this approach, the land-use and ecotoxicity and metal depletion impacts weigh very little compared to other impacts, but the human toxicity impact is significant. In this method, the human toxicity impacts of the composite tanks are lower than the impacts of the steel tank. This is caused by the fact that the ReCiPe method uses the more extensive library of impacts of the USEtox method instead of the recommended one used in the ILCD method. This includes emissions of heavy metals, which dominate the overall impact and are larger for the steel life cycle.

It is easy to understand that the impacts of composite tanks are lower than the impacts of steel tanks, and that the impacts of the Akulon fuel lock lined tanks are slightly lower than the impacts of HDPE lined tanks because of the effect of weight reduction on fuel consumption in cars.

The only significant impact category for which this is not certain is human toxicity.

The energy flows to be reported are included in table 5 below.

Flow	Unit	Steel	HDPE	Akulon
Cumulative energy demand	MJ	10,511	6,821	6,034
Renewable energy consumption	MJ	0	35	34
Non-renewable energy consumption	MJ	10,511	7,057	6,259

Table 5: Energy flows

The energy flows follow a similar pattern to the environmental impacts.

5. Quality assessment

5.1. Quality management

5.1.1. Data quality indicators

In table 6, the data quality indicators, in accordance with the pedigree table recommended by the WBCSD guideline are included. The pedigree matrix gives a description for each quality level from 1 to 5, 1 meaning high quality and 5 meaning very low quality.

Life cycle stage	Item	Technological representativeness	Geographical representativeness	Time representativeness	Completeness	Reliability
Materials production	Steel	2	2	4	1	2
	Glass fibre	2	2	1	1	2
	Epoxy resin	2	2	3	1	2
	Akulon fuel lock	1	1	1	1	2
	HDPE	2	2	3	1	2
Tank manufacture	Type 4 tanks	4	2	3	3	2
	Steel tank	3	2	3	3	2
Use	Transport emissions	2	1	1	1	2
	Methane emissions	1	1	1	1	1
End of life	Incineration of type 4 tanks	2	2	3	3	3

Table 6: Data quality indicators

As the transport emissions and methane emissions dominate the differences in impact, the data quality is critical for these items, and indeed, they get the best scores.

5.1.2. Cut-off

All known elementary flows in the system boundary have been included. It cannot be excluded that certain elementary flows are unknown or not included in models for upstream processes. However, it is hard to imagine that such small omissions would affect the conclusions of this study.

5.1.3. Data management plan

The critical parameters in this study are the permeability of HDPE for methane and the transport emissions. Transport emissions go down gradually over time, and HDPE permeability can be affected by the grade. The results of this study are valid for at least five years provided there is no new form of HDPE with a lower permeability.

5.2. Uncertainties

5.2.1. Qualitative description of uncertainties

Only uncertainties in methane permeation and in transport emissions are critical for the conclusions of this report. As demonstrated in section 5.1.1, the quality of the permeability data is very good and the quality of the transport emissions data is good. Therefore uncertainties are relatively low.

5.2.2. Quantitative uncertainty assessments

The uncertainty in methane permeation measurement results is well within 10%. Therefore there is a maximum uncertainty of 10% in the magnitude of the advantage of Akulon fuel lock lined tanks over HDPE lined tanks. This uncertainty does not affect the conclusions of this study.

The fuel consumption dependence on weight that was used in this study is a gross oversimplification of reality. This dependence is strongly dependent on many parameters, which are affected by engine and vehicle design and driving style. Even when this dependence would be a factor of two lower, Akulon would still score better than HDPE and much better than steel.

Therefore the conclusions drawn from the results are not sensitive to the critical uncertainties in the data.

5.3. Sensitivity analysis

Methane permeation in reality may be different from the permeation measured in the laboratory. But most deviations (for example, because permeation would be affected by a different geometry or in material under stress) would work in the same direction for both liners, meaning that permeation through the Akulon fuel lock liner is certainly lower than the permeation through the HDPE liner.

The uncertainty in transport emissions depends a lot on the fuel efficiency of the vehicle, which depends, among others, on the vehicle weight. This effect is included in the calculation in the first place. The uncertainty is assumed to be about 20%. Therefore, there is an uncertainty of 20% in the magnitude of the advantage of type 4 tanks over metal tanks, but the advantage is certainly there.

Methodological choices can also affect results. The methodological choices in this study are fully in line with the WBCSD guidelines and hence, with ISO 14040:2006 and 14044:2006 standards. Nevertheless, it reinforces the conclusions, if it can be shown, that the results would not be affected by other choices.

The allocation choices in the modelling of refineries will affect the difference between the scenarios studied in this scenario. But because the main effect is a reduction in fuel consumption, this will affect the magnitude of differences but not what is the best solution.

The full recycling scenario chosen for steel is very conservative; any deviation from full recycling will only increase the footprint of the steel cylinder and make the conclusion of this study more pronounced.

5.4. Critical/peer review

This report and study was reviewed by Dave Morris, senior LCA consultant, DSM. This study contains comparative assertions, but as they are not intended to be disclosed to the public, no panel was assigned for the review.

6. Conclusion

The environmental effects of using an Akulon fuel lock lined type 4 compressed natural gas tank compared to metal or HDPE lined tanks are clearly explained. The reduced fuel consumption caused by weight reduction in replacing steel compressed natural gas tanks with composite ones leads to a significant reduction in environmental footprint. In case an HDPE liner is used, the effect on global warming is compensated by the effect of methane permeation through the liner. The Akulon fuel lock liner does not have this disadvantage.

7. References

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PlasticsEurope eco-profiles as implemented in ecoinvent 2.

Case study two

Quantifying the environmental performance of metal replacement with engineering thermoplastics: An LCA case study on LED heat sinks

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Report Date: October 25, 2013

The study has been conducted according to the requirements of *Life Cycle Metrics for Chemical Products: A guideline by the chemical sector to assess and report on the environmental footprint of products* and according to ISO 14044:2006 and ISO 14040:2006 standards.

The detailed methodological report can be obtained from the commissioner.

1. Scoping

1.1. Goal and scope definition

This study was commissioned by SABIC and was completed in-house by the internal LCA team. The objective of this study is to assess the environmental performance/implications of the choice of different materials, such as metals and engineering resins, for energy-efficient and low-carbon emission fabrication of the heat sink part in an LED lighting application.

LEDs are energy efficient, breakage resistant and compact, and they have a long life, making them a sustainable lighting solution. According to a US Department of Energy forecast, LEDs are expected to represent 74% of U.S. general illumination lumen-hour sales by 2030, contributing to an annual primary energy savings of 3.4 quads (or 996,482,200,000 kilowatt-hours) in lighting (U.S. Department of Energy, 2012).

Cost of production is a key impediment to the growth of LEDs. Heat sinks – integral to the efficacy and longevity of an LED – constitute a significant portion of this cost. SABIC's Konduit compounds are a cost-effective, resource-efficient heat sink solution that can contribute to the scaling of LEDs. Traditionally, heat sinks have been made from die cast aluminium. The LNP Konduit compound from SABIC Innovative Plastics is a potential material solution for the solving of thermal conductivity challenges. These compounds boost productivity compared to die cast aluminium, which requires secondary operations and has low yields. The electrically isolating property of Konduit eliminates extra housing, offers 30 percent lighter weight, eliminates the need for painting for surface aesthetics, and enables 3D design freedom to optimise the heat transfer function compared to a heat sink made from die cast aluminium.

The goal of the study is to assess the environmental performance of a heat sink made from a polymer compound with an aluminium insert against a heat sink made from die cast aluminium. The assessment was done through a cradle-to-grave LCA of a 7W LED heat sink having conventional thermal conductivity of die casted aluminium compared to a hybrid solution consisting of a plastic thermal conductive material of a polymer compound with an aluminium alloy insert. To obtain a clear and accurate picture of the entire life cycle of the specified LED heat sink and to account for the recycling of metals at the end-of-life, the scope of this study was selected as a cradle-to-grave assessment. Figure 4 shows the heat sink made from hybrid Konduit and a heat sink made from die cast aluminium.

The study has been conducted following guidelines of ISO 14044:2006 standard. For life cycle modelling, the SimaPro V7.3.3 software was used.

Figure 4: Heat sink made from Konduit and heat sink made from die cast aluminium

1.1.1. Intended application(s) of the study

The aim of this study is to provide a basis for considering sustainability as one of the key decision factors during the choice of materials at the product design stage. The results of this LCA study will be a first step towards establishing the potential environmental benefits of metal replacement by engineering thermoplastic resins targeting engineering properties like thermal conductivity and electrical isolation.

1.1.2. Reasons for carrying out the study

The study aims to help customers make environmentally informed choices in thermal conductive material alternatives when assessing and implementing improvements, such as changes in product, process and design, raw material use, industrial processing and waste management.

1.1.3. Business goal

The business goal of this LCA study is to establish the environmental and performance benefits of thermoplastic heat sink materials and position these new innovative products as an alternative solution to traditional metal heat sinks for key customers in emerging LED lighting applications. This also helps in developing value chain collaborations to identify next generation heat sink material needs.

1.1.4. Target audience

The LCA results are communicated mainly to product designers and customers from the lighting industry with interest in engineering plastics with special properties, such as thermal conductivity and electrical isolation. The study is also recommended for internal and external stakeholders and technical experts dealing with environmental decision support related to products and resources.

5.2. System boundaries

1.2.1 System boundaries description

The main system boundary for the product system for aluminium and polymer hybrid heat sinks is given in figure 5.

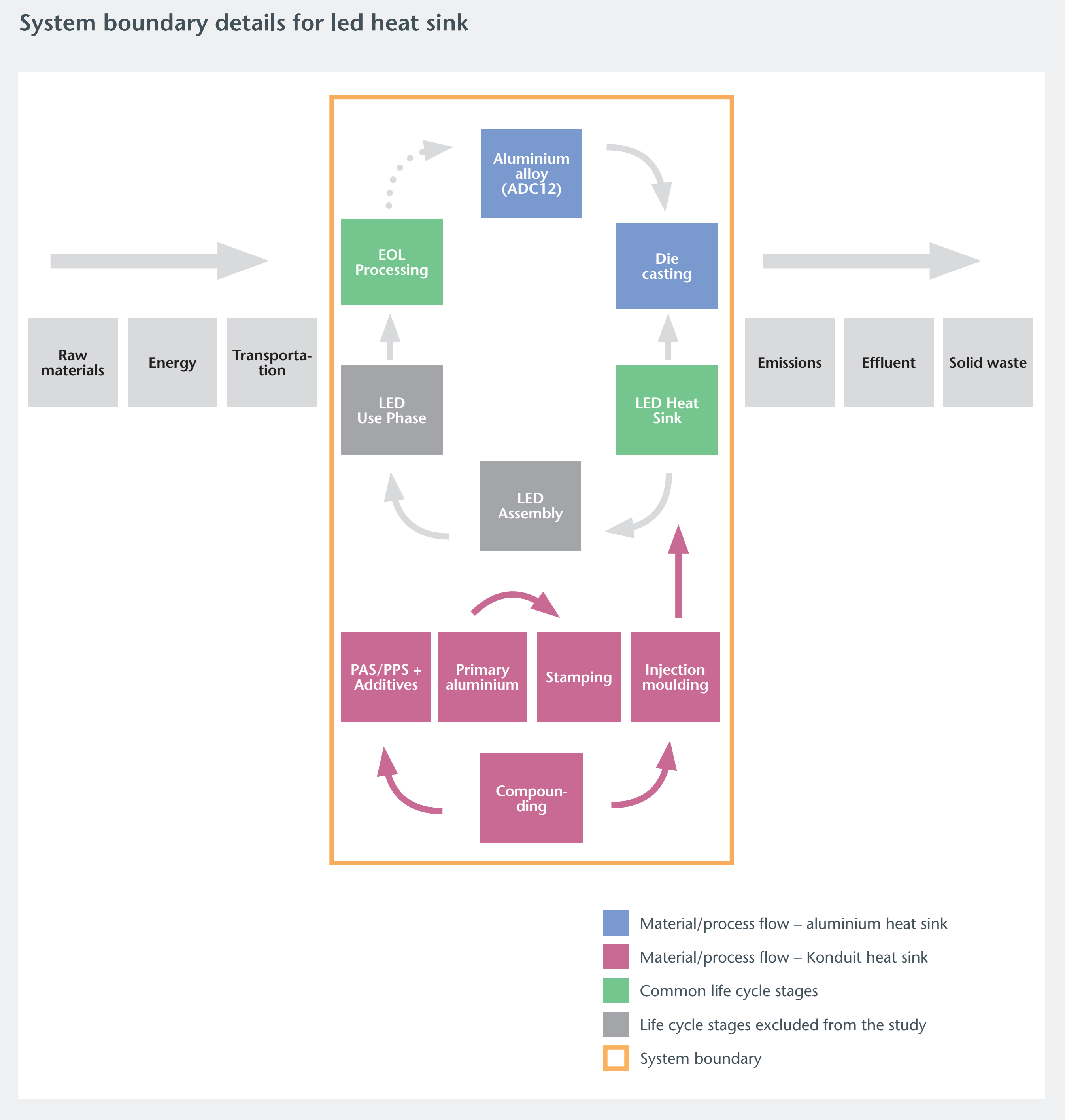

Figure 5: System boundary details for LED heat sink

The product system includes the following life cycle stages:

- Raw material extraction/acquisition;
- Material processing;
- Product manufacturing;
- Final disposal/end-of-life (EOL).

As China is the leading country for the manufacturing of LEDs (Gereffi and Lowe), the geographic boundary of manufacturing LEDs was assumed as 80 percent from China and 20 percent from Europe. The location of the use phase, end-of-life and any other process was Europe.

Temporal boundaries of the study are defined from 2012 to 2016, the period representing the majority of data collected.

1.2.2. Limitation statement

LED assembly and use phases were excluded from this study since these phases are assumed to be equivalent for the two product systems.[14] The study has been conducted for a 7W LED heat sink as a pilot; other wattages have not been included.

1.3. Functional unit

1.3.1. Function description

Heat sinks are enclosures used to dissipate heat from a heat source and prevent the overheating of the source. Heat sinks are essential in dissipating the heat generated from an LED chip, which if not dissipated can reduce the lifetime of an LED. The temperature of the LED chip must be maintained at 75-85°C,[15] otherwise the life span of the LED is reduced exponentially.

1.3.2. Functional unit description

The functional unit of this case study has been selected as one unit of heat sink to dissipate heat from a 7W LED source during 50,000 hours of use guaranteeing a temperature of 75-85°C for the LED chip. The functional unit has been selected based on the same intended use and same lifetime for a 7W LED.

1.3.3. Comparability statement

To ensure the comparability of the lifetime of the two different heat sinks, one made from aluminium and one a Konduit hybrid, the temperature has been taken as a reference parameter. Internal thermal analysis shows a 2 to ~5℃ difference in temperature for both heat sinks. A temperature difference of up to 5℃ in heat sinks can be considered as having the same lifetime. The same analysis has been validated with the customer.

In addition to functional features, such us thermal conduction, the Konduit hybrid heat sink has additional features such as an electrical isolative and increased resource efficiency over an aluminium heat sink. System boundary, allocation procedure and end-of-life options are considered as the same for both product systems.

1.3.4. Duration of the functional unit

A typical lifetime of 50,000 hours[16] has been taken as service life for the 7W LED under study.

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[14] Application knowledge from the customer

[15] http://www.allledlighting.com/author.asp?section_id=3021&doc_id=560157

[16] http://www.vossloh-schwabe.com

2. Methodological choices

2.1. Choices for impacts and flows

The life cycle impact assessment (LCIA) was carried out for the following impact categories, as per *Life Cycle Metrics for Chemical Products: A guideline by the chemical sector to assess and report on the environmental footprint of products.*

Impact categories

- Global warming
- Photochemical ozone formation
- Air acidification
- Abiotic depletion (element)
- Eutrophication (marine and freshwater)
- Human toxicity and ecotoxicity
- Dust and particulate matter
- Land use
- Ozone depletion

Energy and other flows

- Cumulative energy demand
- Renewable energy consumption
- Non-renewable energy consumption
- Land occupation

The details of impact categories and intermediate flows with units and methodologies used for this study are given in table 7.

Impact category	Impact category indicator	Methodology	Comments
Global warming potential	kg CO_2 eq.	IPCC 2007 GWP 100a V1.02	
Photochemical ozone formation	kg Ethylene eq.	CML 2 baseline 2000 V2.05	
Air acidification	molc H+ eq.	ILCD 2011 Midpoint V1.01	
Mineral, fossil and renewable resource depletion	kg Sb eq.	ILCD 2011 Midpoint V1.01	
Eutrophication (freshwater)	kg P eq.	ILCD 2011 Midpoint V1.01	
Eutrophication (marine)	kg N eq.	ILCD 2011 Midpoint V1.01	
Human toxicity	CTUh	ILCD 2011 Midpoint V1.01	Human toxicity (cancer effects)
Human toxicity	CTUh	ILCD 2011 Midpoint V1.01	Human toxicity (non-cancer effects)
Ecotoxicity	CTUe	ILCD 2011 Midpoint V1.01	Freshwater ecotoxicity
Dust and particulate matter	kg PM2.5 eq.	ILCD 2011 Midpoint V1.01	
Land use	kg C deficit	ILCD 2011 Midpoint V1.01	
Ozone depletion	kg CFC-11 eq.	ReCiPe Midpoint (H) V1.07	
Cumulative energy demand	MJ	Cumulative Energy Demand V1.08	
Renewable energy consumption	MJ	Cumulative Energy Demand V1.08	
Non-renewable energy consumption	MJ	Cumulative Energy Demand V1.08	
Land occupation	m^2a	ReCiPe Midpoint (H) V1.07	Agricultural land occupation and urban land occupation

Table 7: Impact categories and intermediate flows

Lack of CML methodology implemented in the software led to the reporting of mineral, fossil and renewable resource depletion (kg Sb eq.) from the ILCD 2011 Midpoint V1.01 instead of resource depletion (fossil fuels) and abiotic depletion (element) as mentioned in the guidance. Species richness is excluded as per the decision tree on the impact categories mentioned in the guidance. This impact category is not a priority for the stakeholders, is not currently practiced in LCA studies, and there is a lack of methodology implementation in the LCA software.

Note that water footprint is not reported for this LCA study due to a lot of uncertainty in water data quality and ongoing developments in water footprint methodology. However, the gate-to-gate water withdrawal data for products is available on request.

2.2. Allocation rules between co-products

This section is not relevant for this LCA case study.

2.3. Attribution of recycling benefits

Allocation procedures used in this study for aluminium is "open-loop with closed-loop recycling" based on ISO/TR 14049:2000 (ISO 2000). This procedure is applicable where recycling in a product-specific system participates in product independent material pools, such as recycled glass, steel, aluminium, etc. The product-specific system delivers secondary raw material into that pool and is supplied with secondary material by the pool. The recycling credit is credited back to the product system as per the recycling allocation, followed by the aluminium industry alloy recycling loop as shown in figure 6.

Recycling loop for aluminum alloy (Hoberg)

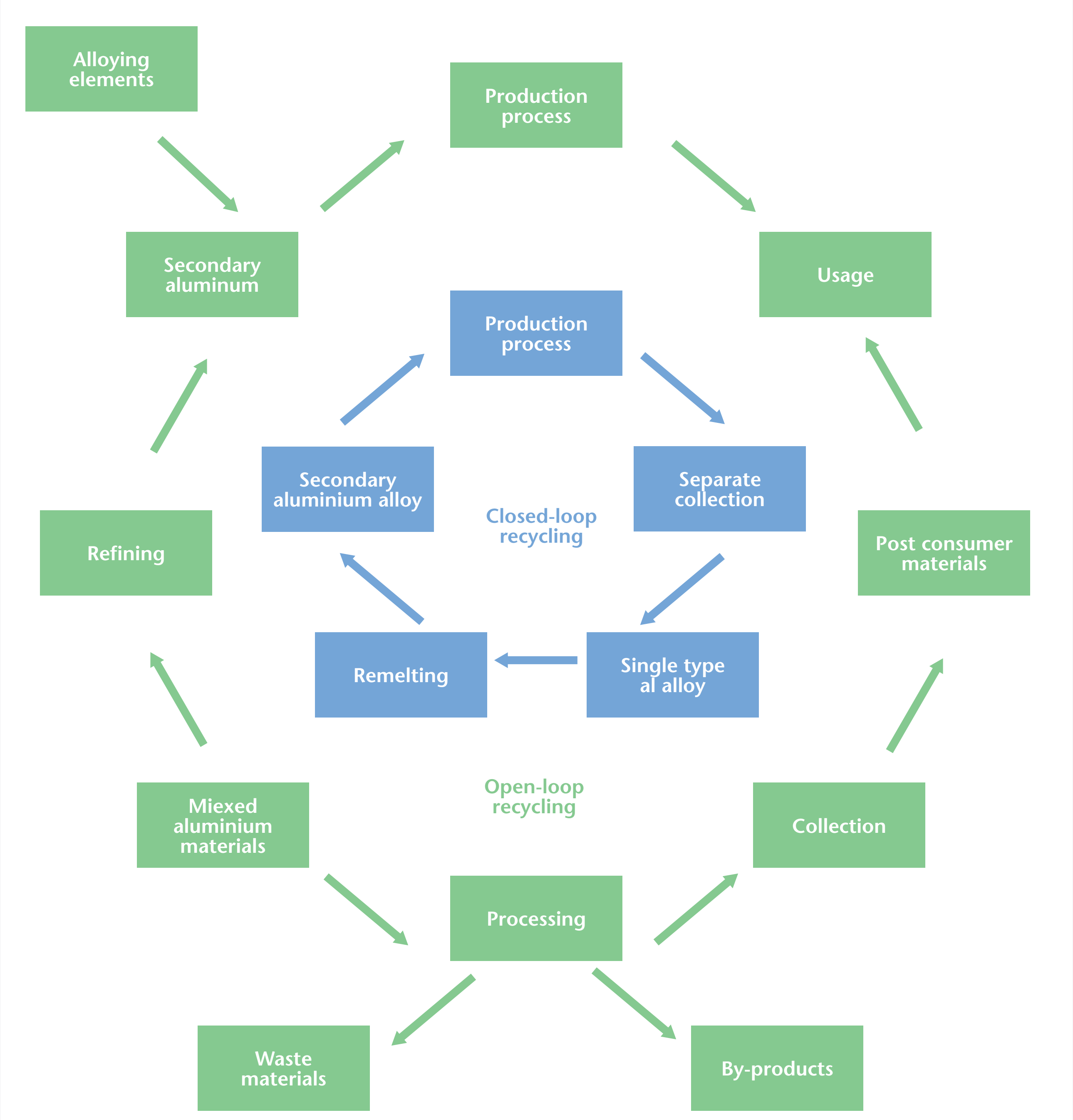

Figure 6: Recycling loop for aluminium alloy (Hoberg)

For the polymer part of the Konduit product system, the energy recovered from incineration is credited back to the product system as per the avoided burden approach.

2.4. Avoided emissions

This section is not relevant for this LCA case study.

2.5. Biogenic uptake and emissions

This section is not relevant for this LCA case study.

2.6. Carbon storage and delayed emissions

This section is not relevant for this LCA case study.

2.7. Direct land-use change / indirect land-use change

This section is not relevant for this LCA case study.

3. Data sources

3.1. Life cycle inventory analysis procedures

The specifications used for polymer hybrid and die casted aluminium heat sinks are given in table 8. The specifications have been collected from different product suppliers' data and SABIC's application development sources.

Material	Volume (m^3)	Density (g/cm^3)	Weight (g)
Polymer	2.1E-05	1.6	34.1
Aluminium insert	4.6E-06	2.7	12.4
Aluminium heat sink	2.6E-05	2.7	68.5

Table 8: Specifications for heat sinks made from polymer hybrid and aluminium

The details of different process yields and scrap rates for both product systems are provided in table 9.

Process	Yield	Scrap %	Scrap - fate
Injection moulding	98%	2%	Landfill
Sheet making	~100%	~0%	Lost
Stamping	72%	28%	Internal recycling
Die casting	45%	50%	Internal recycling

Table 9: Process yield and scrap rate

The material balance for both product systems is given in table 10.

Material flow for heat sink made from die casted aluminium	
Initial material used	152 g
Post-industrial recycled (PIR)	41%
Post-consumer recycled (PCR)	30%
Loss	29%
Material flow for heat sink made from Konduit	
Initial material used	52 g
PIR (aluminium)	9%
PCR (aluminium)	16%
Landfill	37%
Incineration with energy recovery	6%
Loss	32%

Table 10: Material balance

3.2. Data sources description and data used

Koduit material is a ready-to-mould thermoplastic commercially available from SABIC that consists of polyamid/polyphenylene sulphide (PA/PPS)-based resin plus some additives. The inventory for making the base resin is collected from recent plant data. The inventory includes raw materials inputs, utilities, process emissions and effluent details to make the base resin. All background data was selected from the latest ecoinvent data set available in the Simapro software. All missing or incomplete inventory details were collected through LCI from material suppliers, own-plant LCI data and recent published literature. In the case of some of the additives, the information was neither available in the Simapro software nor in the open literature; therefore these were excluded from the modelling based on the relevance and mass cut-off criteria (<1 percent based on mass).

Fabrication of heat sink made from Konduit compound with aluminium insert

The average European industry data set for plastic injection moulding is used for the fabrication of a polymer hybrid heat sink, and a 98% yield is used for the injection-molded part as per the data set.

The aluminium alloy (5052-H32) composition details for the insert are collected from openly available literature (The Aluminum Association 2009 and ASM Aerospace). Since the recycling credit is taken back to the system, the aluminium part of the alloy inventory started with primary aluminium instead of a production mix. The data set for sheet rolling of aluminium is used for the sheet-making process. The loss/yield of the sheet-making process is ignored. as it is not going to make much difference in the final results. For sheet fabrication, a 72% process yield (Debreuil et al, 2010) has been taken. The post-industrial recycled (PIR) part is considered to be recycled and the credit is taken back as aluminium alloy to the product system as per the recycling allocation.

The end-of-life scenario for a heat sink made from polymer hybrid is assumed as waste electrical and electronic equipment (WEEE) disposal. The heat sinks are assumed to be recovered from the waste stream and sent to the WEEE recycling facility. The recovery and recycling rate is taken as an average value for lighting equipment for Western European countries available on the European Union (EU) website.[17] The balance is assumed to be lost or unrecovered and will finally end up in landfill. The end-of-life burdens include impacts arising due to disposal of materials and energy consumption in reprocessing (dismantling (Hischier et al. 2005), shredding, etc.), transportation of scrap materials (Alston and Arnold 2011) and other EOL process for energy recovery and recycling.

A conservative approach to incineration with energy recovery and landfill at a 50:50 ratio (European Chemicals Agency 2001 and PlasticsEurope 2009) is assumed for plastic heat sink. As per the avoided burden approach, the energy recovered from incineration is credited back to the product system. The post-consumer recycled (PCR) aluminium from an end-of-life of polymer hybrid heat sink is recycled and the credit has been given back to the system as per the recycling loop (Hoberg) given in figure 6. Due to high uncertainty around the composition of aluminium alloys in the waste stream and to the fact that the secondary aluminium produced from the processed material is of varying quality as per market demand, the end-of-life credit has been given separately as primary aluminium and alloy metals.

Fabrication of a heat sink made from die cast aluminum

The aluminum alloy ADC12[18] (equivalent to AA383) is used to make the aluminum heat sink. No cut-offs were applied during the inventory analysis. The inventory details for aluminium casting alloy have been collected from open literature.[19] Due to data variations found in openly available literature for the die casting yield, PIR and loss from casting, average values are taken from the literature. The die casting yield, PIR and loss are taken as 45%, 50% and 5% respectively (Tharumarajah et al. 2009 and Neto 2008).The energy and other utilities details are taken from various literature (Tharumarajah et al 2009).[20] End-of-life recycling, recovery rate, transportation, sorting and dismantling energy have been taken to be the same as polymer hybrid heat sink as a WEEE at the disposal site. The PIR and PCR are modelled separately. The existing ecoinvent data set for recycling of aluminium is used for foundry scrap as well as PCR recycling. PIR from the die-casting process and the PCR from the EOL recycling are credited back to the product system as per the recycling allocation with reference to the aluminium alloy recycling loop (figure 6). The PIR and PCR credit has been taken as similar to aluminium alloy (5052-H32) in the hybrid heat sink product system.

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[17] See http://epp.eurostat.ec.europa.eu/portal/page/portal/waste/key_waste_streams/waste_electrical_electronic_equipment_weee

[18] http://zskaibo.en.alibaba.com/product/422596842-210647100/aluminum_die_casting_led_housing.html and http://www.ledlinearlighthousing.com/product_detail_ID_323.htm

[19] See http://www.vossloh-schwabe.com and http://www.alibaba.com/product-gs/209984065/ADC12_aluminum_alloy.html

[20] See http://www.alibaba.com/product-gs/209984065/ADC12_aluminum_alloy.html

4. Results and interpretation

Figures 7 and 8 show the comparative results from the cradle-to-grave LCA of heat sinks made from die casted aluminium with a heat sink made from polymer hybrid for global warming potential (GWP) and cumulative energy demand (CED) (includes non-renewable (NR) and renewable (R) energy part) respectively.

The figures show that the raw material production impacts of both GWP and CED are high for heat sinks made from die casted aluminium due to its relative high mass compared to heat sinks made from polymer hybrid. Primary aluminium production processes like extraction, refining and smelting, etc. led to high energy use and greenhouse gas (GHG) emissions. As compared to aluminium, the study shows that a polymer hybrid heat sink results in 78% lower emissions and up to 79% lower energy consumption during the raw material manufacturing phase.

Fabrication impacts for both GWP and CED are high for heat sinks made from die casted aluminium due to the 45% yield of the die casting process as compared to an injection moulding yield of 98%, which leads to higher material and energy usage at the fabrication stage. Typically an injection-moulding machine will use 1.2-2.2 kW/kg of polymer processed, whereas die casting uses 3.2 kWh/kg of aluminium processed. As compared to aluminium, the study shows that Konduit results in 71% lower emissions and up to 66% less energy consumption during the fabrication phase. The approach to modelling end-of-life in this study is open loop with closed loop recycling. Therefore the impacts of this phase include EOL benefits as well as burdens. The EOL benefits include credit from the recycling of metal and recovery of energy through the incineration of polymer waste. The EOL burdens include impacts arising due to energy consumption in reprocessing (sorting, separation, incineration and re-melting), transportation of scrap materials, and loss or disposal of material that ends up in landfill.

In the case of heat sinks made from die casted aluminium, approximately 86% of material is recovered and recycled throughout the lifetime, and about 14% of the material is assumed to end up in landfill. The recovered material displaces the need to manufacture virgin metal, and is therefore considered an EOL benefit. In the case of heat sinks made from a polymer hybrid, the EOL benefit is 50% energy recovery from the incineration of the material recovered. Since the EOL benefits are directly proportional to the weight of the material recovered, aluminium has the highest benefit in this phase. This is because of the relatively higher recovery and recycling potential for aluminium. A heat sink made from die casted aluminium has 85% higher GWP benefit and 86% higher CED benefit as compared to heat sinks made from a polymer hybrid.

The overall comparison of each heat sink's cradle-to-grave life cycle stages reveals that the polymer hybrid heat sink has up to 68% lower GWP and CED as compared to the die casted aluminium heat sink. Although the aluminium heat sink received more credit at EOL due to the higher recyclability of metal, the assessment shows an overall higher impact for aluminium due to the relatively higher weight and lower fabrication yield of the aluminium heat sink, leading to more raw material usage.

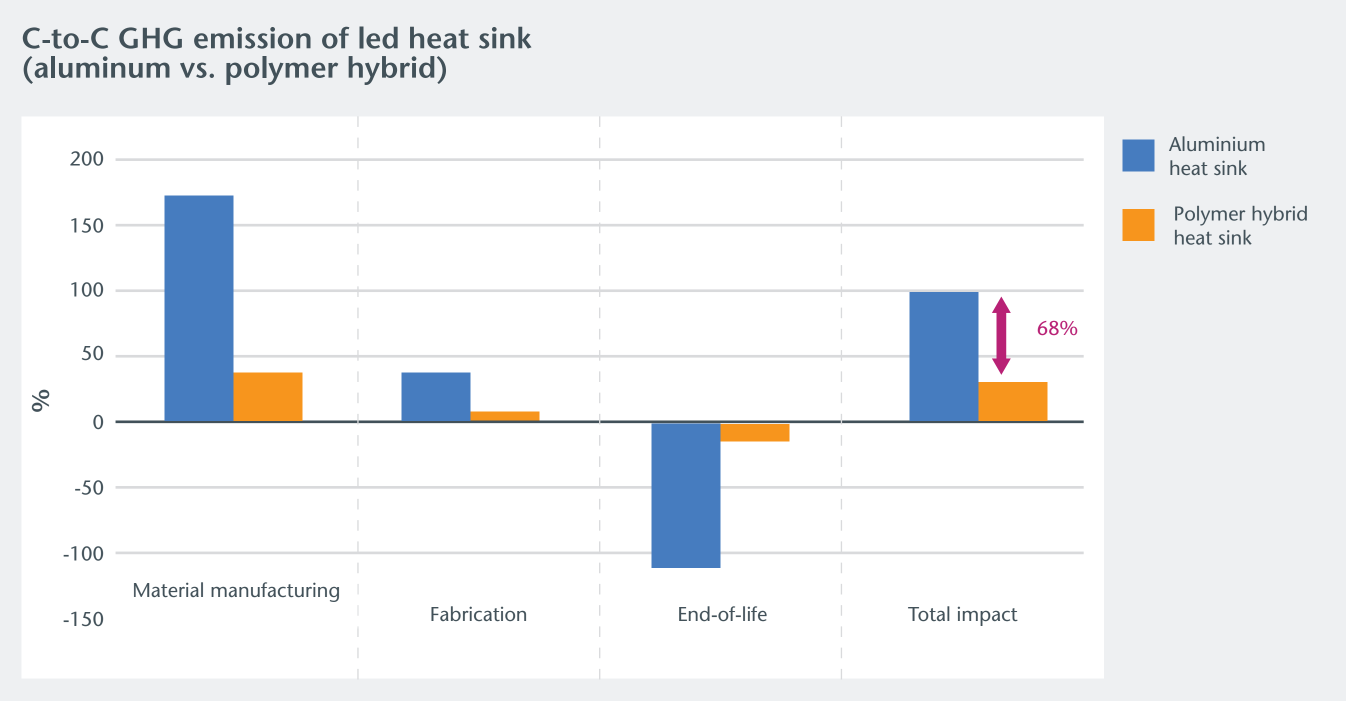
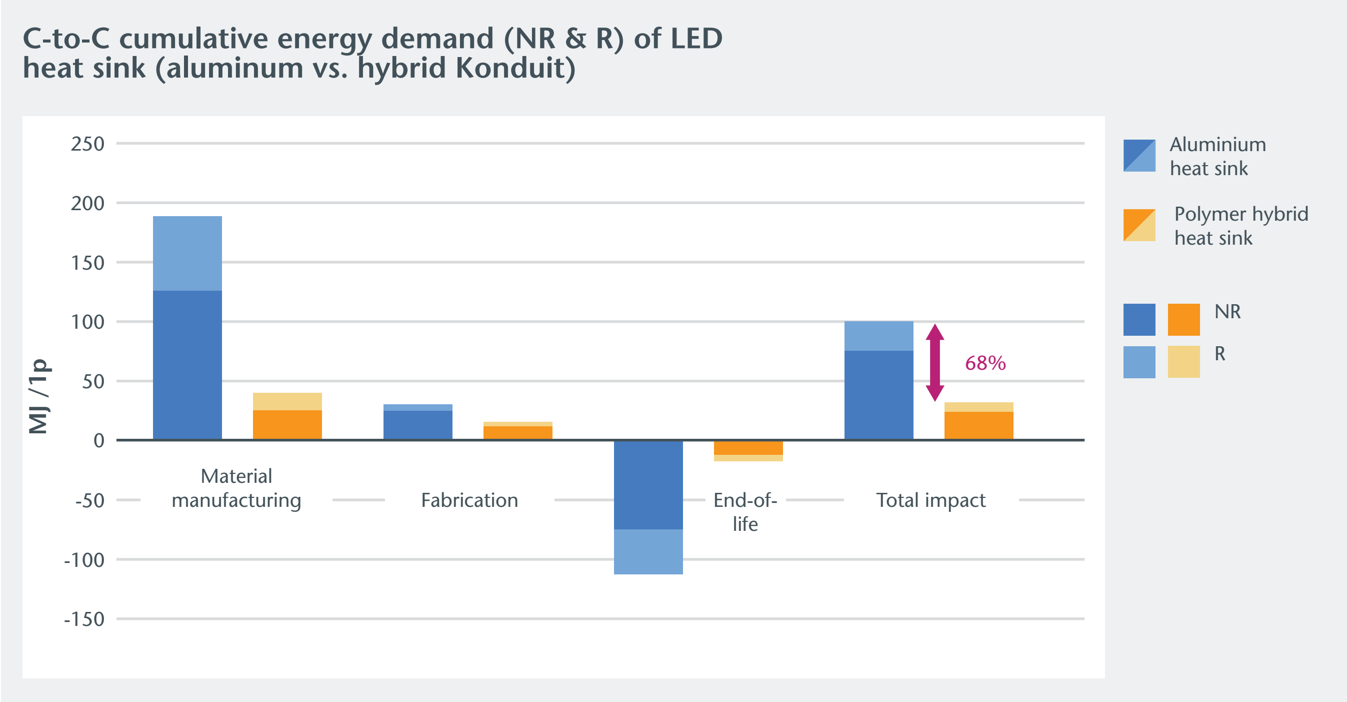


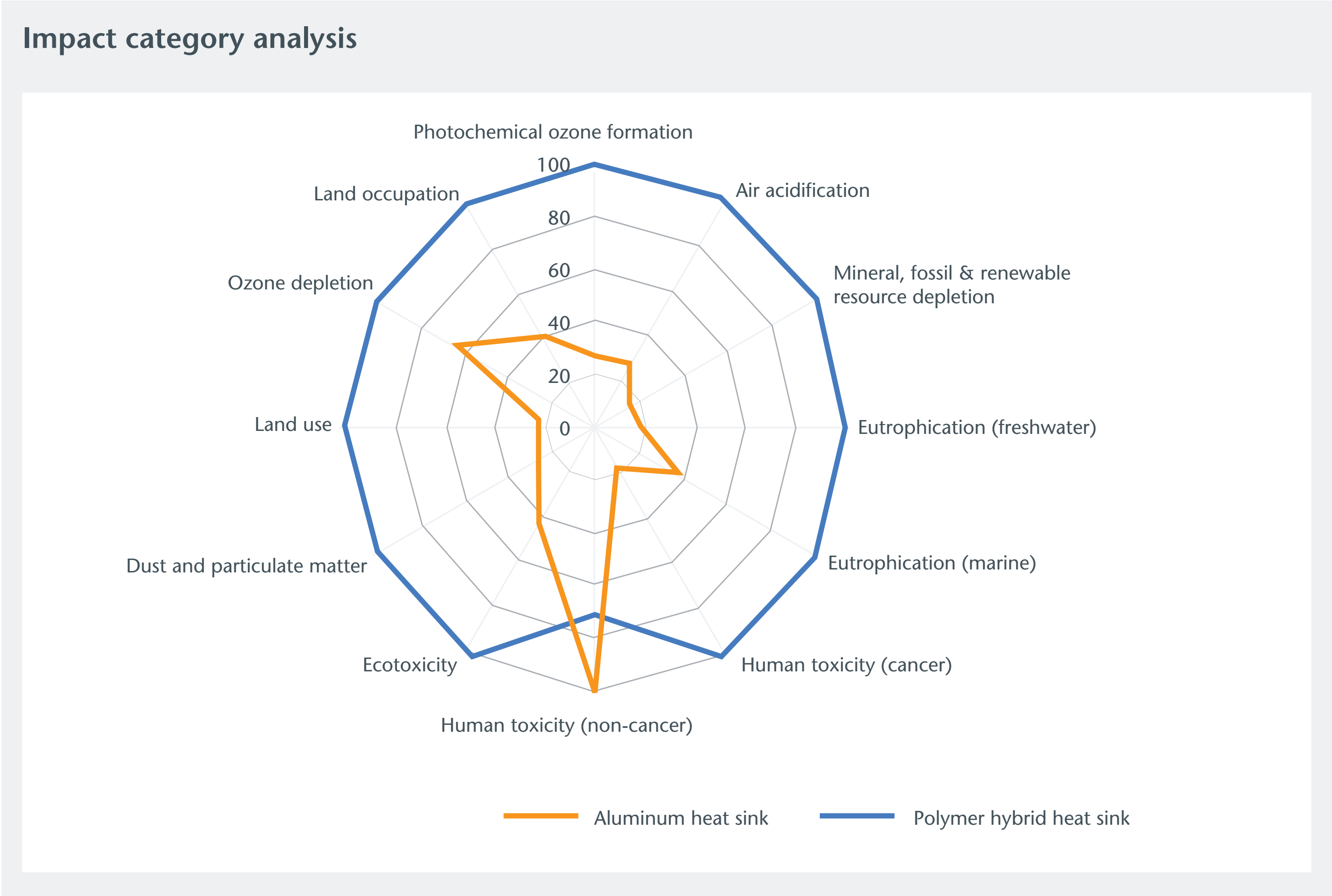
Figure 7: GWP - heat sink made from die casted aluminium and heat sink made from Konduit hybrid



C-to-C cumulative energy demand (NR & R) of LED heat sink (aluminum vs. hybrid Konduit)

Figure 8: CED - heat sink made from die casted aluminium and heat sink made from Konduit hybrid

Figure 9 shows the results for other impact categories and intermediate flows mentioned in table 2 other than GWP and CED (NR and R). Analysis of the figures shows that a heat sink made from Konduit hybrid has a lower impact in all impact categories, except human toxicity (non-cancer effects), compared to a heat sink made from die casted aluminium.



Impact category analysis

Figure 9: Impact category analysis - heat sink made from die casted aluminium and heat sink made from Konduit hybrid

This results section includes the entire impact category and energy flows as mentioned in section 2.1. The results are relative to the goal and scope of this study as mentioned in section 1.1. These results are directly related to the life cycle inventory and characterisation factors that have been applied in order to obtain the impact assessment results to facilitate the interpretation.

5. Quality assessment

5.1. Quality management

5.1.1. Data quality indicators

The uncertainty analysis is done by using Monte Carlo analysis. The uncertainty of each input data set is specified by a pedigree matrix of six different uncertainty factors. Data sources are assessed according to six characteristics: reliability, completeness, temporal correlation, geographic correlation, further technological correlation and sample size. All the background data sets from ecoinvent carry some uncertainty factors from the data set provider. All data sets are assumed to have lognormal distribution as the probability distribution.

5.1.2. Cut-off

Mass cut-off criteria (<1 percent based on mass) has been applied for some inventory wherever no details are available. No energy cut-off criteria have been used.

5.1.3. Data management plan

This study should remain relevant for at least five years. A detailed unit process inventory and details for each life cycle stage have been documented in a separate Excel file. This will make it easier to account for any changes or upgrades for data inventory in the future.

5.2. Uncertainties

Each input data set uncertainty is accounted for with a pedigree matrix and the uncertainty is calculated with Monte Carlo analysis. Each product life cycle is run for thousands of iterations to perform the uncertainty analysis. Figures 10 and 11 show the comparison of uncertainty analysis of GWP and CED for heat sinks made from die casted aluminium and polymer hybrid. The figures show that by considering all data variations and uncertainty, there is a clear difference between the product systems at even a 95 percent confidence interval. And it shows that the Konduit heat sink has a lower footprint compared to the aluminium heat sink at all variation levels.

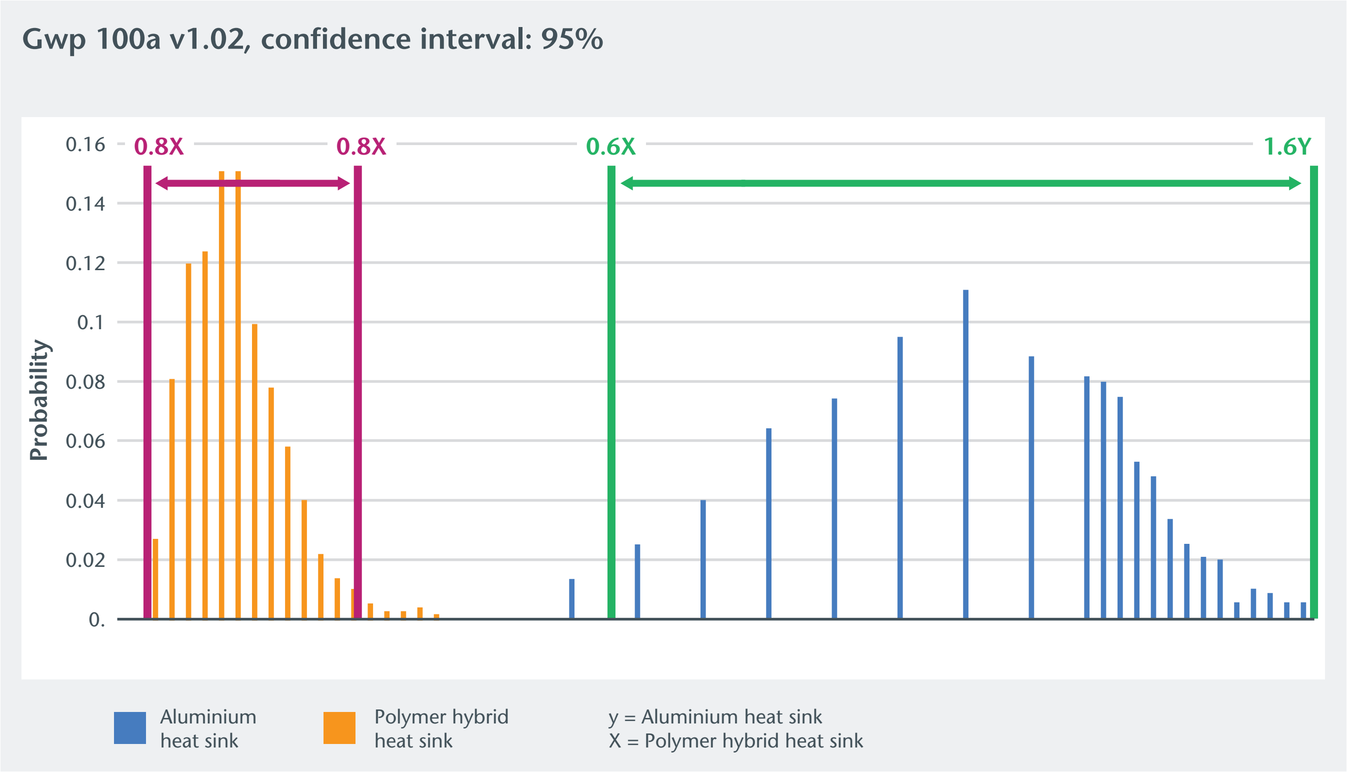


Figure 10: Uncertainty analysis of 1 p aluminium heat sink and 1 p polymer hybrid heat sink for GWP

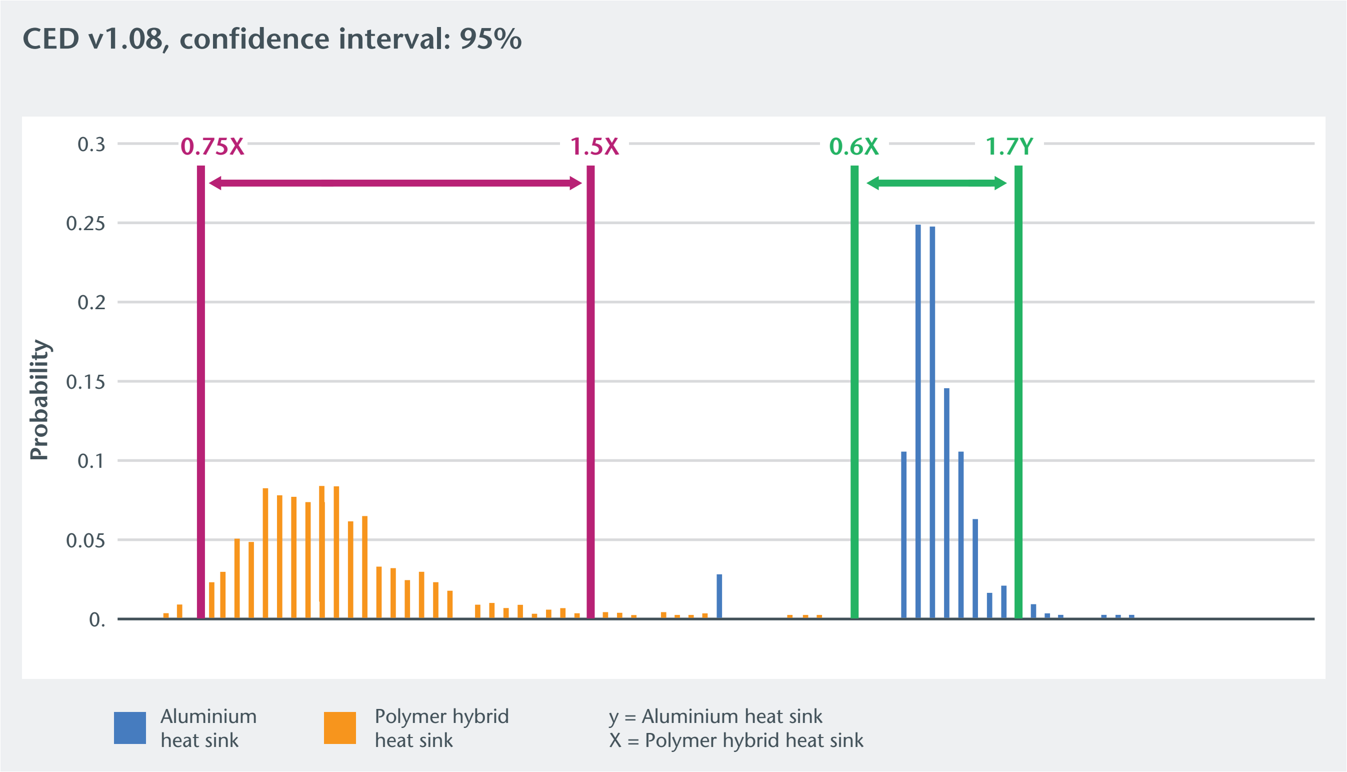


Figure 11: Uncertainty analysis of 1 p aluminium heat sink and 1 p polymer hybrid heat sink"for CED.

5.3. Sensitivity analysis

The following sensitivity parameters were used to assess the variation in results due to different modelling choices and method assumptions for a die casted aluminium heat sink and a polymer hybrid heat sink. Aluminium best case (selecting all the potential best parameters together) and Konduit product system worst case (selecting all the potential worst parameters together) sensitivity was performed to scope the boundary of the results. Note that all these best and worst case scenarios will not all happen together in real life application. Results are given in figures 12 and 13 for GWP and CED.

1. Variation in aluminium die-casting yield
2. Variation in aluminium EOL recovery rate
3. Variation in aluminium EOL recycling rate
4. Variation in Konduit EOL recovery rate
5. Variation in Konduit EOL recycling rate
6. Variation in Konduit compounding efficiency
7. Variation in Konduit EOL scenario
8. Variation in material for aluminium heat sink
9. Aluminium best case vs. Konduit worst case

The detailed sensitivity analysis illustrates the robustness of the LCA model, results and final conclusions. In all the sensitivity cases, the Konduit hybrid heat sink shows relatively lower GWP and CED vs. the aluminium heat sink, even in an aluminium best case vs. Konduit worst case scenario.

5.4. Critical/peer review

All the results have been reviewed by an internal review committee for assumptions, methodology and quality of work.

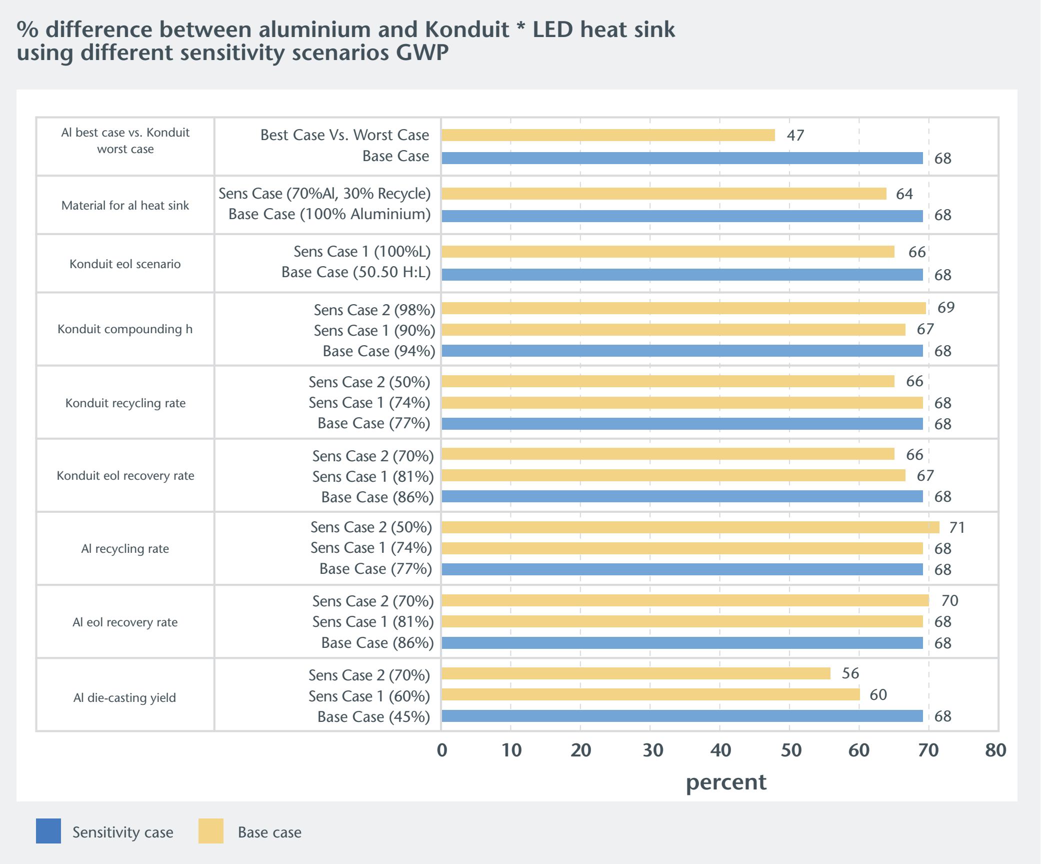


Figure 12: Heat sink made from die casted aluminium and heat sink made from Konduit hybrid comparison using different sensitivity scenarios – GWP

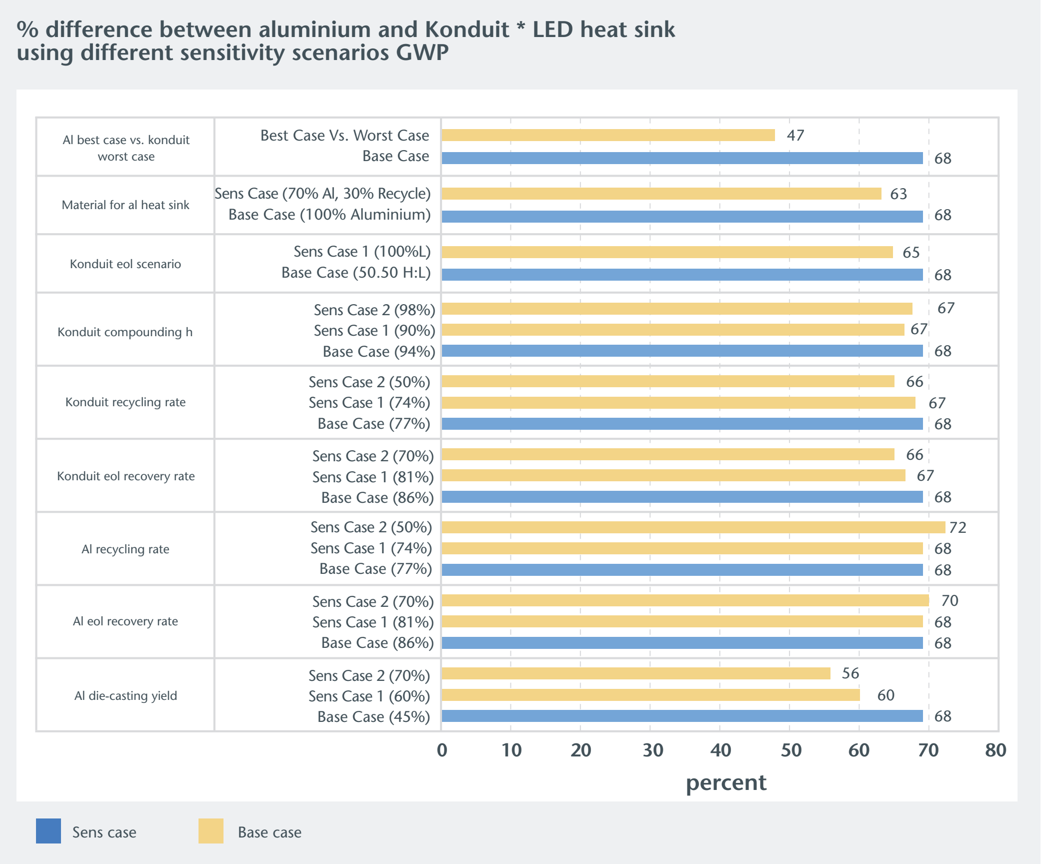


Figure 13: Heat sink made from die casted aluminium and heat sink made from Konduit hybrid comparison using different sensitivity scenarios – CED

6. Conclusion

The life cycle impact assessment (LCIA) study shows that, compared to a heat sink made from die casted aluminium, a heat sink made from Konduit has a significantly better environmental profile in all the key categories. On a per unit heat sink basis, Konduit hybrid has 68% lower GWP and CED than that of die casted aluminium. As mentioned earlier, the aim of this study was to provide a basis for considering sustainability as one of the key decision factors during the choice of materials at the product design stage. This LCIA study will be a first step towards establishing the potential environmental benefits of metal replacement by engineering thermoplastic resins targeting engineering properties such as thermal conductivity and electrical isolative.

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The WBCSD provides a forum for its 200 member companies - which represent all business sectors, all continents and a combined revenue of more than $7 trillion - to share best practices on sustainable development issues and to develop innovative tools that change the status quo. The Council also benefits from a network of 60 national and regional business councils and partner organizations, a majority of which are based in developing countries.

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