LCA Compendium – The Complete World of Life Cycle Assessment

Series Editors: Walter Klöpffer · Mary Ann Curran

Andreas Ciroth
Rickard Arvidsson *Editors*

Life Cycle Inventory Analysis

Methods and Data

Springer

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Aims and Scope

Life cycle assessment (LCA) has become the recognized instrument to assess the ecological burdens and human health impacts connected with the complete life cycle (creation, use, end-of-life) of products, processes, and activities, enabling the assessor to model the entire system from which products are derived or in which processes and activities operate. Due to the steady, world-wide growth of the field of LCA, the wealth of information produced in journals, reports, books, and electronic media has made it difficult for readers to stay abreast of activities and recent developments in the field. This led to the realization of the need for a comprehensive and authoritative publication.

LCA Compendium – The Complete World of Life Cycle Assessment discusses the main drivers in LCA (SETAC, ISO, UNEP/SETAC Life Cycle), the strengths and limitations of LCA, the LCA phases as defined by ISO standards, specific applications of LCA, Life Cycle Management (LCM) and Life Cycle Sustainability Assessment (LCSA). Further volumes, which are closely related to these themes will cover examples of exemplary LCA studies ordered according to the importance of the fields of application. They will also present new insights and new developments and will keep the whole work current. The aim of the series is to provide a well-structured treatise of the field of LCA to give orientation and guidance through detailed descriptions on all steps necessary to conduct an LCA study according to the state of the art.

LCA Compendium – The Complete World of Life Cycle Assessment anticipates publishing volumes on the following themes:

- Background and Future Prospects in Life Cycle Assessment (published in March 2014)
- Goal and Scope Definition in Life Cycle Assessment (published in September 2016)
- Life Cycle Inventory Analysis (LCI) – Methods and Data (published 2021)
- Life Cycle Impact Assessment (LCIA) (published in March 2015)
- Interpretation as well as, Critical Review and Reporting in Life Cycle Assessment (in print 2021)
- Special Types of Life Cycle Assessment (published in July 2016)
- Life Cycle Management (LCM) (published in August 2015)
- Life Cycle Sustainability Assessment (LCSA)
- Life Cycle Assessment Worldwide

More information about this series at http://www.springer.com/series/11776

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Preface

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Not just since the Fridays for Future movement, which began August 2018, but since decades, foresighted public policy making, corporate supply chain management and product development rely on an environmental life cycle perspective. Governments, administrations, and companies use the results of environmental life cycle assessments of packaging materials, fuels based on renewable materials, or of their full supply chains to identify hotspots, improvement potentials, and new regulatory measures.

Two elements of the life cycle inventory (LCI) analysis are key for the reliability and quality of the outcomes of an LCA (life cycle assessment): the system model and the life cycle inventory data. Similar to a civil engineer, who uses a simplified model to dimension the load-bearing structure of a building, the LCA practitioner designs a simplified system model to represent the product system under analysis that is suited for the goal for which the LCA is carried out. Rosenblueth and Wiener (1945) claimed in their paper on the role of models in science that "the best material model for a cat is another, or preferably the same cat." This is not practical but tempting. Increasing both the geographic and time resolution of LCIs, for instance, is a challenge for the model design. The art of parsimonious model design which helps to address the most pressing environmental issues and eliminate the main causing industrial or agricultural activities is to capture the characteristics of the object of investigations and its supply chains, which are relevant in relation to the goal and scope of the LCA. This is where brainpower should replace simplified mechanistic models on one hand and time and computing power needed to establish overly complex system models, and to calculate the environmental footprints of products, services and organizations on the other.

*Rolf Frischknecht, jointly with Reinout Heijungs, has been the founder of the volume "Life Cycle Inventory Analysis". He created the nucleus and developed the fundamentals of the concept. Finally, he delegated his responsibility as editor to Andreas Ciroth and Rickard Arvidsson who further developed the concept and brought the volume to finalization. See also chapter 4 of this volume "Multi-functionality in Life Cycle Inventory Analysis: Approaches and Solutions" by Jeroen Guinée, Reinout Heijungs and Rolf Frischknecht.

Once the appropriate system model is ready, appropriate LCI data is needed. While LCI data was hardly publicly available in the infancy of LCA (1970–1990), the first material, comprehensive, consistent, topical, transparent, and quality controlled LCI databases were established, further developed, and expanded in the last 30 years (Frischknecht et al. 1994, 2004). The LCI datasets offered in these databases address those human activities that are causing a large share of societies' impact on the environment (materiality). They cover a broad set of elementary flows and include capital goods (comprehensiveness); follow a strict set of modeling guidelines, including allocation and electricity mix modeling (consistency); use most recent information as far as possible, feasible, and available (timeliness); are reported on a unit process gate to gate level which allows for a duplication of the LCI results (transparency, see also Frischknecht 2004); and are reviewed by an external independent third party (quality control). In addition, LCI data must represent real situations, and the documentation in a dataset must refer to its LCI data (reality check). Third parties should be able to crosscheck the references used to establish a certain amount of input or a certain emission factor reported in the dataset. Despite all these characteristics and requirements, the LCI datasets offered remained fairly simple and clear.

In all those years since the dawn of unified LCI databases, the following controversial discussions were loyal companions of LCI database operators and LCA practitioners:

a) Allocation and recycling: credits or no credits – that is the question. Credits are tempting, but they challenge inter-generational equity and fair environmental competition.
b) Attributional or consequential: it is a dream to quantify the environmental impacts caused by decisions. However, it is very difficult, if not impossible, to establish stringent causal relationships between an individual decision and the impacts it causes, unless the decision is about a really big thing. While simple and mechanistic rules were used in the past (Ekvall and Weidema 2004), consequential LCAs nowadays make use of general and partial equilibrium models and plug in traditional LCAs (e.g., Igos et al. 2015).
c) Process-based or input-output based LCA: while precision versus completeness dominated the debate on the more appropriate approach in the past, the two approaches are subsequently used to quantify the supply chain of environmental impacts of organizations. Input-output based assessments are carried out, firstly, to identify potential hotspots within the supply chains of organizations. Secondly, process based LCA is then used to identify improvement potential within the hotspot areas.

The task of LCI experts and LCI database providers resembles the work of a ferryman: it is a service to life cycle practitioners, with recurring tasks of regularly updating LCI data of the same or similar commodities and with recurring methodological discussions. In that sense, this type of work has a meditative character. At the same time, this work is of utmost importance because LCI databases are the core foundation of many, if not all, LCAs and their conclusions and recommendations. A solid LCI foundation is a necessary but not a sufficient prerequisite for solid LCAs with solid recommendations in view of a society that strives to live within the boundaries of our planet Earth.

This book *Life Cycle Inventory Analysis – Methods and Data* is a milestone in the history of LCI methodology and analysis and of LCA in general. It gives an excellent overview on the current state of discussions and technical developments and possibilities. I am convinced that it will help to generate and maintain robust and appropriate LCI data and models suited to address the multiple pressing environmental challenges we face.

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Chapter 1
Introduction to "Life Cycle Inventory Analysis"

Rickard Arvidsson and Andreas Ciroth

Abstract This chapter introduces the life cycle inventory (LCI) analysis – the topic of this volume. A brief history of the concept is provided, including its procedure according to different standards and guidance books. The LCI analysis phase of the life cycle assessment (LCA) framework has remained relatively constant over the years in terms of role and procedural steps. Currently, the LCI analysis is situated in between the goal and scope definition phase and the life cycle impact assessment phase in the LCA framework, although it is interconnected also with the interpretation phase. Central concepts in LCI analysis are defined, including product system, process, flow, functional unit, and system boundary. Four important steps of LCI analysis are outlined: constructing a flow chart, gathering data, conducting calculations, as well as interpreting results and drawing conclusions. The focus is on the process LCA approach, which is the most common in LCA practice. Environmentally-extended input-output analysis is also described briefly. Finally, an overview of the other chapters of this volume and their relevance to the topic of LCI analysis is provided.

Keywords Allocation · Data gathering · Environmentally-extended input-output analysis · Inventory · Life cycle assessment (LCA) · Life cycle impact assessment · Life cycle inventory analysis (LCI)

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1 A Brief History of Life Cycle Inventory Analysis

An important role of life cycle assessment (LCA) is to contribute to sustainable product development. In order to do so effectively by assessing negative environmental consequences and trade-offs with other sustainability aspects, an LCA study needs "to be as quantitative as possible" (Klöpffer 2003). Since the first attempts to formalize the life cycle assessment (LCA) framework, life cycle inventory (LCI) analysis has been a central part. No wonder, because in order to conduct a quantitative environmental assessment, obtaining quantitative data related to the object of study is crucial, and this is a core step of LCI analysis. In fact, the LCI analysis might be older than the LCA framework itself, of which it is currently seen as a part, considering early accounts of life cycle energy requirements at an inventory level in the 1970s (Hannon 1972; Makhijani and Lichtenberg 1972). Despite its long history, the definition and procedure of the LCI analysis has remained relatively constant over time, although some details vary between different sources.

In the early work on LCA (1970–1990), the LCI analysis was sometimes considered to contain the definition of goal and scope (Vigon et al. 1993). One of the earliest attempts to harmonize the LCA framework was conducted in the Code of Practice by the Society of Environmental Toxicology and Chemistry (SETAC) (Consoli et al. 1993). In this work (and onwards), the LCI analysis phase is seen to be separate from the goal and scope definition (Fig 1.1a). The steps included in the LCI analysis according to the Code of Practice are: (1) defining systems and system boundaries; (2) creating process flow charts; (3) gathering, calculating, and reporting data; and (4) conducting allocation (if coproducts or recycling processes exist in the system). It is further described that all inputs and outputs for which data has been found should be scaled to the functional unit of the study, which is still common practice in LCA today.

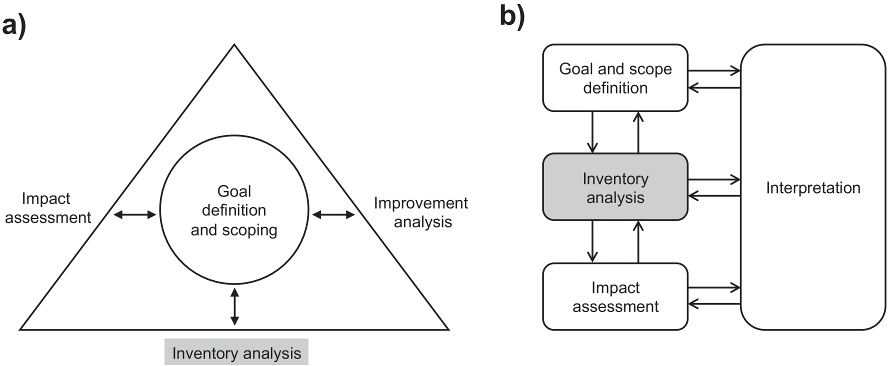

Fig. 1.1 Life cycle assessment frameworks from SETAC's Code of Practice (Consoli et al. 1993) (**a**) and from the most recent ISO standard (2006) (**b**), with the life cycle inventory analysis phase highlighted in gray in both cases

The Nordic Guidelines on LCA from 1995 state that the LCI analysis contains the following steps, where, in particular, (1) and (2) are similar to (1) and (3) in SETAC’s Code of Practice, respectively: (1) Description of the product system (functions and boundaries), (2) data collection and calculations, as well as (3) a sensitivity and uncertainty assessment (Lindfors et al. 1995). In an early handbook on LCA, Boguski et al. (1996) outline five steps of LCI analysis: (1) define the scope and boundaries, (2) gather data, (3) create a computer model of the product system studied, (4) analyze and report the study results, and (5) interpret the results and draw conclusions. The first two steps are similar to those in the Nordic Guidelines. An 8 years newer textbook provides a different set of three steps for conducting an LCI analysis, where step (2) about data gathering is common between the two books: (1) construction of the flow chart, (2) data collection, and (3) calculation of emissions and resource use (Baumann and Tillman 2004). Although SETAC’s Code of Practice, the Nordic Guidelines and the two books use somewhat different wording, they convey a similar procedure in practice and several of the steps are shared almost literary between these guidance texts.

The most recent 2006 ISO standard for LCA, as well as the previous ISO standard from 1997, provide the currently widely accepted framework for LCA, with the LCI analysis placed in between the goal and scope definition and the life cycle impact assessment (LCIA) phases (Fig 1.1b). The 2006 standard states that the LCI analysis phase includes “data collection and calculation procedures to quantify relevant inputs and outputs of a product system.” It specifically lists three important steps of an LCI analysis: (1) data collection, (2) data calculation, and (3) allocation of flows and releases, where the last step can be seen as a specific type of calculation. These three steps can be recognized in several of the previously cited sources, such as SETAC’s Code of Practice (all three), the Nordic guidelines (the first and second), and the textbook by Baumann and Tillman (2004) (the first and second).

As all phases in the current LCA framework, the LCI analysis is iterative and connected to the other phases (ISO 2006). Typically, the LCA analyst learns more about the system under study during the LCI analysis, which can sometimes have implications for the other phases. For example, if data is found to be exceptionally scarce during the data gathering of the LCI analysis, the goal and scope of the study might have to be redefined. The analyst might then need to lower the ambition of the study in different ways, for example, by reducing the number of included impact categories. The other phases of the LCA framework might also warrant a revisiting of the LCI analysis. For example, if the LCIA phase shows strange or even unreasonable impact results, the LCI analysis might have to be revisited to improve the data coverage and/or quality. The LCI analysis is thus an integrated part of the LCA framework and procedure rather than an isolated step to be ticked off.

2 LCI Analysis in a Nutshell

The ultimate purpose of the LCI analysis is generally to use the inventory data result in the subsequent LCIA step for calculating environmental impacts by using the following equation (Hauschild and Huijbregts 2015):

$$IS_j = \sum_i \sum_k \sum_l Q_{i,k,l} CF_{j,i,k,l} \tag{1.1}$$

where *IS* stands for impact score (e.g., climate change), CF stands for characterization factor, *Q* stands for the quantity of emission or resource use from the inventory, *i* is a certain contributor (emission or resource) to the impact category *j*, *k* is the location of the emission or resource use, and *l* is the environmental compartment to which the emission occurs or from which the resource is extracted.

Before describing how to conduct an LCI analysis to obtain emission and resource use quantities *Q*, a number of important concepts need to be defined. These entities are shown in italic below and their definitions are modified from those in the ISO standard (2006). The very object of study in an LCI analysis is the *product system*, which is a set of processes that are connected by energy and/or material flows. In addition, the product system must perform one or more of the functions outlined in the goal and scope definition phase. *Processes*, in turn, are nodes in the societal metabolism where flows meet and can be transformed. A *unit process*, specifically, is the least aggregated process level in the product system. Unit processes are thus the building blocks of a product system, much like brick stones are building blocks of walls. The above-mentioned *flows* are movement of energy and/or materials, which can be of different types. *Outputs* are flows that leave a process, whereas *inputs* are flows that enter a process. Examples of outputs are emissions to the environment (air, water, or soil), by-products, waste, and flows that enter other processes for further handling. Inputs can be resources from the environment or flows from upstream processes in the product system. *Elementary flow* is a specific term for flows leaving or entering the natural environment. The *functional unit* is the quantified performance of the product system, which is the reference unit to which all flows are scaled in the LCI analysis phase. The *system boundary* is the border between a product system, the natural environment, and other product systems. The system boundary thus delimits the product system to be studied.

In this section, we describe four steps that can be found in guidance documents on LCI analysis (Sect. 1). The first three specifically correspond to those in the textbook by Baumann and Tillman (2004): (1) constructing a flow chart, (2) gathering data, and (3) conducting LCI calculations. In addition, we follow the early handbook by Boguski et al. (1996) and include a fourth step: (4) interpreting results and drawing conclusions.

2.1 Constructing a Flow Chart

A step frequently mentioned in guidance documents on LCI analysis is the construction of a flow chart (Sect. 1). Two simple examples of flow charts are provided in Fig. 1.2. Flow charts depict the processes included in the product system, usually represented by boxes, as well as material and energy flows within the product system, usually represented by arrows. When constructing a flow chart, the analyst typically departs from the product or main (foreground) system studied. The inputs to that system are then identified. Then, the processes from which they originate are identified. For these processes, their inputs are then identified, and so on. The graphical illustration of the result of this procedure is the flow chart. Heijungs (2014) provided the following five useful recommendations for drawing a flow chart:

- Processes are represented by boxes
- Products (including services and waste) are represented by arrows between boxes
- The main direction must be chosen, e.g., from top to bottom or from left to right, although some loops may be present
- Environmental interventions are not shown because the diagram focuses on the structure of the processes
- Numbers are not shown (for the same reason)

Note that we do not follow the fifth recommendation in Fig. 1.2 – numbers are displayed there to facilitate an example calculation later in this section. In real-world LCA studies, such data can indeed preferably be provided outside the flow chart.

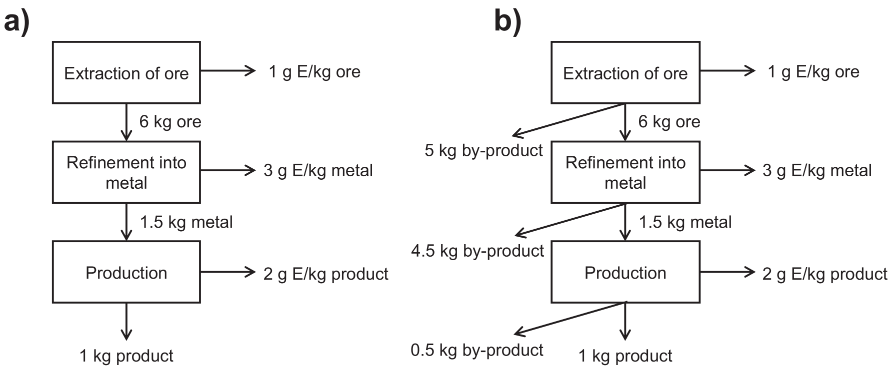

Fig. 1.2 Illustration of two flow charts that can be used to calculate life cycle inventory data results, one without by-products (**a**) and one with by-products (**b**)

2.2 Gathering Data

The LCI analysis is about creating the LCA model, and an evidently crucial part of setting up the model is data gathering. As shown in Sect. 1, this is a core step in most guidance documents on LCI analysis. Specifically, data gathering regards the collection of data for the parameter Q in Eq. 1.1, or for parameters from which Q can be estimated. Inventory data need to be gathered for all the unit processes of the product system (ISO 2006). The LCI analysis is often said to be the most time-consuming and labor-intensive phase of an LCA. For any LCA with more than a few processes readily available in LCI databases, this is probably true.

The exact procedure of data gathering is highly dependent on the type of LCA study as specified in the goal and scope definition, and may therefore vary between LCA studies. Already Consoli et al. (1993) listed a number of potential data sources, including:

- Process designers
- Engineering calculations
- Estimations from similar operations
- Commercial databases

Although formulated almost 30 years ago, these data sources broadly reflect the current LCA practice. Often, a product system is divided into a foreground system of processes central to the studied product (that a certain actor can influence) and a background system of inputs purchased from global markets (that is beyond the influence of a certain actor), a division proposed by Tillman (2000). Additional important sources of data, in particular, for the more in-depth studied foreground system of an LCA, include scientific papers, governmental and industry reports, environmental statistics, as well as various expert judgments. Today, LCA databases provide generic data suitable for the background systems of most studies, see also Chap. 6.

2.3 Conducting LCI Calculations

Regarding the calculations of the LCI analysis, Suh and Huppes (2005) describe that the most common approach is through flow charts. This approach is referred to as process or process-based LCI analysis (Nielsen and Weidema 2001; Rebitzer et al. 2002). By departing from the functional unit of the study, flows are traced backward and forward until they cross the system boundary of the flow chart, at which point the amount of input or output is recorded. The more complicated the product system is, the less simple the calculations become. Complicating factors include processes that produce several output flows or receive several input flows, as well as loops within the system. To illustrate the varying difficulty of conducting an LCI analysis given differently complicated flow charts, Fig. 1.2 shows two

Table 1.1 Example of a simplified unit process for the production process in Fig. 1.2b

Flow	Quantity	Unit
Input		
Metal	0.5	kg/kg product
Output		
Product	1	kg/kg product
By-product	0.5	kg/kg product
Emission E	2	g/kg product

examples, where the data presented can be seen as the result of data gathering activities as described in Sect. 2.2. To make the illustration easy to understand, the two examples include only one generic emission E (corresponding to Q in Eq. 1.1) as output apart from the main product and by-products. The flow charts in Fig. 1.2 show simple, cradle-to-gate product systems. They consist of three unit processes each: extraction of ore, refinement into metal, and production of the product. The data for each of these processes can be expressed as a unit process – Table 1.1 shows a simplified unit process for the production process in Fig. 1.2b. Such unit processes are the building blocks of the process LCI analysis.

Inventory results for emission E (m_E) can then easily be calculated as for the system in Fig. 1.2a:

$$m_E = 2 + 1.5 \times 3 + 6 \times 1 = 12.5\,\mathrm{gE/kg\ product} \tag{1.2}$$

An alternative way to calculate inventory results is using the matrix approach, where the LCI inventory result is a matrix (vector) **M** with the different emissions and resources used in the rows (Suh and Huppes 2005). To calculate **M**, one then needs to define a technology matrix **A** with unit-process input commodities (e.g., crude oil and metal ore) in its rows and processes (e.g., production and use) in its columns. If a commodity is an output to a process, it is given a positive sign (+), and conversely, if a commodity is an input, it is given a negative sign (−). In addition, the matrix **B** is defined to be a matrix containing the emissions and resource use for each process, thus with emissions and resources in its rows and processes on its columns. Finally, **k** is defined as a matrix (vector) containing only the functional unit of the study. The LCI result of the system in Fig. 1.2a can be calculated using the matrix approach as follows, giving the same result as Eq. 1.2:

$$\begin{aligned} \mathrm{M} = \mathrm{BA}^{-1}\mathrm{k} &= \begin{bmatrix} 1 & 3 & 2 \end{bmatrix} \begin{bmatrix} 1 & -4 & 0 \\ 0 & 1 & -1.5 \\ 0 & 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 3 & 2 \end{bmatrix} \begin{bmatrix} 1 & 4 & 6 \\ 0 & 1 & 1.5 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 7 & 12.5 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 12.5\,\mathrm{gE/kg\ product} \end{aligned} \tag{1.3}$$

Since only one generic emission E is considered, the **B** matrix becomes a vector in this example. For more than one type of emission and/or resource use, it would become a nonvector matrix.

One complicating factor mentioned above is the case of several outputs, which can be referred to as the multifunctionality problem in LCA (Guinée et al. 2004). In Fig. 1.2b, the challenge of several output flows is introduced by adding a by-product for each of the processes. Multifunctionality can be handled in different ways. The ISO standard (2006) for LCA mentions three options in order of preference:

1. Avoid allocation by dividing multifunctional processes into subprocesses or expanding the system to include additional functions related to the coproduct
2. Partition between different products based on physical relationships
3. Partition between different products based on other relationships, such as economic value

In addition to these three options proposed by the ISO standard, additional allocation approaches are possible (Majeau-Bettez et al. 2018). The first option mentioned in the standard is often executed through expanding the system to include the use of the by-products and the substitution (disuse) of some other product fulfilling the same function, as described by Weidema (2000). The inventory data of the substituted products are then subtracted from that of the main product. Regarding partitioning based on physical properties, a common example is to partition based on the mass of products:

$$P_{i,mass} = \frac{n_i m_i}{\sum_i n_i m_i} \tag{1.4}$$

where $P_{i,mass}$ is the mass-based partitioning factor, n_i is the amount of product i, and m_i is the mass of the same quantity. Using mass-based allocation, the inventory results from the data in Fig. 1.2b can, with some extra effort, be calculated as:

$$m_E = 2 \times \frac{1}{1+0.5} + 1.5 \times 3 \times \frac{1.5}{1.5+4.5} + 6 \times 1 \times \frac{6}{6+5} \approx 5.7\,\mathrm{gE / kg\ \ product} \tag{1.5}$$

As can be seen, the introduction of by-products reduces the amount of emission allocated to the main product, since the by-products take a share of the burdens.

In partitioning based on economic value, emissions and resource use are often allocated to by-products based on their market price (Guinée et al. 2004). The rationale for using economic allocation is that the economic value often is the main driver behind the production of products and by-products, with the economic value then reflecting the extent to which the by-product causes the production and associated emissions (Ardente and Cellura 2012). Analogous to Eq. 1.4, the economic allocation is conducted as:

$$P_{i,econ} = \frac{n_i x_i}{\sum_i n_i x_i} \tag{1.6}$$

where $P_{i,econ}$ is the economic value-based partitioning factor and x_i is the economic value of product i.

Note that even the flow chart in Fig. 1.2b is much less complicated than those of most LCA studies. In particular, introducing multiple inputs flows to processes and considering loops (e.g., due to recycling) soon make the calculations too complicated to be performed by hand. To aid the calculations of the LCI for such more complicated product systems, different softwares are available to aid the calculations, ranging from spreadsheets in Microsoft Excel to dedicated LCA software such as SimaPro, GaBi, openLCA, Umberto, and CMLCA.

Once the complete LCI has been calculated, results are typically presented in the form of inventory tables. These contain the various emissions and resources used related to the functional unit of the study. In Fig. 1.2 example, only one emission is included, which would make a very short inventory table. Instead, Table 1.2 shows a hypothetical example of an inventory table with more emissions and resources used, including emission E as one among several. Note that in real-world LCA studies, inventory tables are typically much longer.

Table 1.2 Example of an inventory table for a hypothetical case with a functional unit called FU

Flow	Quantity	Unit	Note
Output: Main product			
Product	1	FU	–
Output: Waste			
Solid waste	1700	kg/FU	To landfill
Liquid waste	69	liter/FU	To incineration
Output: Emissions			
Emission A	14	kg/FU	To air
Emission B	0.50	g/FU	To air
Emission C	23	g/FU	To air
Emission D	65	g/FU	To water
Emission E	12.5	g/FU	To water
Emission F	0.21	g/FU	To water
Emission G	4200	g/FU	To water
Emission H	130	mg/FU	To soil
Input: Resources			
Resource R	13	kg/FU	–
Resource S	500	kWh/FU	–
Resource T	4200	kg/FU	–
Resource U	9.8	kg/FU	–
Resource V	2.5	MJ/FU	–

Under "Note," various different types of information can be added, including also data sources

2.4 Interpreting Results and Drawing Conclusions

Although the interpretation of LCA results is generally done after the LCIA phase, some preliminary interpretations can be done already after the LCI analysis. An early hotspot analysis can be conducted to identify the most major energy and materials inputs. For example, in Table 1.2, resource T has the by far largest input flow by mass to the product system. Regarding energy use, resource S seems to be dominating. Aggregated inventory indicators can be applied or developed to facilitate hotspot analysis on an inventory level (see further Chap. 9). For emissions, emission A is the largest contributor by mass (Table 1.2). However, this type of hotspot analysis is of more questionable value for emissions considering their large differences in impact per amount emitted for some impact categories. The toxicity potential is perhaps the most extreme case here, for which differences in impact per amount emitted can be larger than 10 orders of magnitude between substances. The impact of the mass-wise smaller emission E might thus have a much larger toxicity impact than the mass-wise larger emission A.

Another valuable type of interpretation that can be done already at an inventory level is comparing similar product systems to identify differences in inputs and outputs. Such differences can reflect variation in process setup and/or performance, which might become more difficult to identify once the inventory results have been characterized in the LCIA phase. To take a recent example, Furberg et al. (2019) conducted a partial inventory-level comparison between their results for tungsten trioxide (WO_3) production and the results from Syrrakou et al. (2005) (Table 1.3). As can be seen, for the inputs included in the comparison, most are used at similar amounts. The exceptions are sodium hydroxide, where the difference is about a factor of seven, and sulfuric acid, where the difference is about a factor of three. Although the exact reason for these differences was not discovered, it was noted by Furberg et al. (2019) that these two inputs are connected: the sodium hydroxide is partly used neutralize the sulfuric acid. The reason behind the differences could thus be due to different assumptions about the use of sulfuric acid and/or the need for

Table 1.3 Example of an inventory-level comparison between two LCA studies

Input	Furberg et al. (2019)	Syrrakou et al. (2005)
Aluminum sulfate	0.08	0.08
Magnesium sulfate	0.03	0.03
Sodium carbonate	1.2	1.4
Sodium hydroxide	**0.14**	**1.0**
Sodium sulfide	0.07	0.05
Sulfuric acid	**0.56**	**1.4**

Modified from Furberg et al. (2019). The two inputs for which differences are most notable are highlighted in bold. Unit: kg input/kg WO_3

acid neutralization. The comparison thus provides a starting point for deciphering the differences in results.

Another reason for comparing inventory-level results is to investigate whether the same processes have been considered between different studies in cases where this is poorly reported. If the inventory-level inputs and outputs are widely different, there is a high chance that different processes where considered.

3 Environmentally-Extended Input-Output Analysis

Although the process LCI approach described in Sect. 2 is probably by far most common for conducting the calculations of the LCI analysis phase, there is an alternative approach called environmentally-extended input-output analysis (EEIOA) (Nakamura and Nansai 2016; Suh and Huppes 2005). It will not be given much further attention in this book but is described briefly here. The basis for this approach is that there exist economic accounting data worldwide that describes the trade between countries and economic sectors. For example, it is noted in economic accounting when 1000 kg iron ore is imported to the Norwegian construction sector from Sweden. This data thus covers many of the global trade flows. Notably, they also cover flows that are typically not included in the process LCI approach, such as flows related to services, public administration, and social work. Furthermore, some forms of cutoffs are always made in process-based LCI analysis, consciously or not, for example, of inputs that are too minor to show up in the data. The omission of these types of flows in the process LCI approach can be referred to as the truncation problem, which results in a truncation error of the process LCI approach relative to the actual emissions and resources used. This truncation error (ε) can be estimated as (Ward et al. 2017):

$$\varepsilon = 1 - \frac{I_p}{I_{tot}} \tag{1.7}$$

where I_p is the environmental impact as obtained from a process LCI analysis and I_tot is the estimated total impacts. Estimations of the magnitude of the truncation error range from a few percent to as much as 100% of the impacts depending on the product and estimation method (Ward et al. 2017), indicating that the truncation error can indeed be substantial. These estimations support the use of the EEIOA approach since it presumably captures a larger share of the impacts resulting from emissions and resource use. The trade flows can be supplemented with so-called environmental extensions, which relate the economic trade flows to emissions and resource use by assuming a proportional relationship between them. Similar to the matrix representation approach, the EEIOA makes use of matrix calculations. The inventory result is then a matrix (vector) **q** containing emissions and resource use (corresponding to the **M** matrix in Eq. 1.6) associated to a demand **y** (Suh 2004):

$$\mathrm{q} = \mathrm{B}\left(\mathrm{I} - \mathrm{A}\right)^{-1} \mathrm{y} \tag{1.8}$$

where **B** is a matrix containing all emissions and resources used (corresponding somewhat to the **B** matrix in Eq. 1.6), **I** is the identity matrix (with ones in its diagonal and zeroes elsewhere), **A** is a matrix with the inputs to sectors (having sectors both as rows and columns, corresponding somewhat to the **A** matrix in Eq. 1.6), and **y** is a matrix (vector) containing the final demand (corresponding to the functional unit or reference flow of the study, as well as to the **k** vector in Eq. 1.6).

It is possible to use the process LCI analysis approach for the foreground system of a study, where the access to detailed data is often higher, and the EEIOA for obtaining inventory data for background processes. This is referred to as hybrid LCA (Nakamura and Nansai 2016; Suh 2004; Suh et al. 2004; Hendrickson et al. 2006). With such an approach, the final demand **y** is not set to the reference flow of the entire study, but to a certain input to the foreground system from the background system. An example could be an input of electricity or a chemical such as ethanol. The emissions and resource use (the **q** vector) are then calculated for that specific input, rather than taking the background system data from e.g. an LCA database.

In addition to avoiding truncation errors, the EEIOA approach has the advantage of being faster – it can be used to conduct an LCA study within a few hours (Hendrickson et al. 2006). There are several EEIOA databases available, most notably EORA, EXIOBASE, WIOD, GTAP-MRIOT, GRAM, and IDE-JETRO (Tukker and Dietzenbacher 2013). However, not all countries are typically covered in these databases underpinning the EEIOA approach to LCI analysis, but some are rather aggregated into larger regions, such as "rest of the world Asia and Pacific" and "rest of the world Africa." Some economic sectors can also be much broader than individual products, such as "forestry products" and "textiles." The EEIOA approach thus has both benefits and drawbacks compared to the process-based LCI analysis approach.

4 Overview of this Volume

This volume of the LCA Compendium contains a number of chapters addressing central aspects to LCI analysis.

In Chap. 2, the general principles of setting up an LCI model and LCI analysis are described in more detail by introducing the core LCI model as a relatively simple, linear model, and extensions that allow addressing reality better.

Chapter 3 regards the development of unit processes, which can be seen as the very cells or atoms of LCI analysis. As shown in Chap. 3, developing unit processes of high quality and transparency is not a trivial task but is crucial for high-quality LCA studies.

Chapter 4 regards the multifunctionality problem mentioned in Sect. 2.3.

In Chapter 5, the quality of data gathered and used in LCI analysis is discussed. State-of-the-art indicators to assess data quality in LCA are described and the fitness for purpose concept is introduced: data quality is not an absolute property of a dataset, but instead depends on the application.

Chapter 6 follows up on the topic of LCI data and provides a state-of-the-art description of LCI databases. It describes differences between foreground and background data, recommendations for starting a database, data exchange, and quality assurance concepts for databases, as well as the scientific basis of LCI databases.

The algorithms of LCI analysis are described in Chap. 7 providing the mathematical models underpinning the LCI.

In Chap. 8, the use of LCI data to create aggregated environmental indicators is described. Such indicators include the cumulative energy demand and various water use indicators. These have the advantage of being simple and robust, but at the same time have the disadvantage of being less connected to actual impacts than midpoint or endpoint indicators used in LCA (see further Hauschild and Huijbregts (2015) for a description of midpoint and endpoint indicators).

Chap. 9 links the LCI analysis phase to the subsequent LCIA phase. A clear and relevant link between these phases is crucial since LCI data that does not fit into existing LCIA models will remain unused, and similarly, if no LCIA models exist which fit the LCI data gathered, it too will remain unused. Only with a clear link between them, an LCA study can make use of all the gathered data.

We, therefore, hope this volume provides a good starting point for anyone interested in a thorough description of the LCI analysis phase and its most central aspects.

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Chapter 2
Principles of Life Cycle Inventory Modeling: The Basic Model, Extensions, and Conventions

Andreas Ciroth, Francesca Recanati, and Rickard Arvidsson

Abstract The basic model of a life cycle inventory (LCI), with unit processes as smallest modeling entities, emerged already in the very early phases of life cycle assessment (LCA) method development. It is a rather simple, linear model, with a distinction between elementary flows, product flows, and waste flows. Since the early applications, this simple model proved to be very useful and allowed for various expansions. For certain issues related to LCI modeling, solutions and approaches have evolved as extensions of the basic model. Such issues and related modeling challenges include: the multifunctionality problem; the modeling of loops in product systems; the modeling of the use phase; the modeling of transport services; the consideration of time and long-term emissions in LCI; the definition of the boundary between the technosphere and biosphere; and how to address accidents, incidents, and risks. This chapter presents and explains the basic LCA model and its extensions, where some are commonly used in practice today, and some others not. Furthermore, conventions regarding the modeling of transport services, use phase and products, end of life, are presented.

Keywords Accidents · Biogenic carbon · Biosphere · ISO standards · Life cycle inventory (LCI) model · Multifunctionality · Risks · Technosphere · Use phase

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1 The Basic Life Cycle Inventory Model

The concept of a life cycle is at the core of life cycle assessment (LCA) and of life cycle inventory (LCI) models, which, in the end, aim at modeling impacts of anthropogenic, "man-made" product systems to the environment. The impacts modeled are those linked to one product, which is followed from cradle to grave, that is, from resource extraction to its end of life. The interventions of this anthropogenic system are basically inputs and outputs, as shown in Fig. 2.1. "The environment" can be understood here in a wider sense than merely as environmental impacts, covering everything that is around the anthropogenic system investigated. It is convenient to classify the inputs and outputs of the system further. Inputs can be categorized into resources and other inputs. Outputs can be categorized into emissions to different environmental compartments (air, water, and soil), waste, and products, which are not released to the environment but used by consumers or further processed within the anthropogenic system (Fig. 2.2).

All these inputs and outputs are summarized under the term *flows*. The *product* is one of the flows; it plays a central role since it represents the benefit delivered by the system and can be seen as the reason why the system exists at all. Demand for the product created in the system triggers the resource needs and the emissions of the system. The anthropogenic system is often referred to as the *technosphere*, and its surrounding is referred to as the *biosphere* (Milsum 1968).

A *life cycle* is commonly divided into several life cycle stages, such as raw material extraction (or acquisition), manufacturing and production, distribution and transport, use and maintenance, as well as finally recycling and treatment of waste (Fig. 2.3). Considering the whole life cycle is often mentioned as key to avoid burden-shifting and to evaluate a product in a comprehensive manner (ISO 2006a; Bjørn et al. 2018), and it is at the core of the LCI modeling, as well as LCA as a whole.

The life cycle is built from, and consists of, processes that are linked by exchanging products. This means that products are delivered from one process to the next, while causing emissions and contributing to resource extraction. The product or products of the entire life cycle is/are described in terms of a functional unit. It is common that the same product from the same process occurs as an input (and/or output) several times in a life cycle, for example, electricity and transport. Figure 2.4 shows this schematically, with the product system being incomplete due to potential

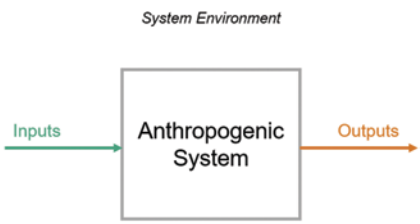

Fig. 2.1 Most basic model of life cycle inventory modeling: an anthropogenic system with interventions to the environment, as inputs and outputs. (Fava et al. 1991, adapted)

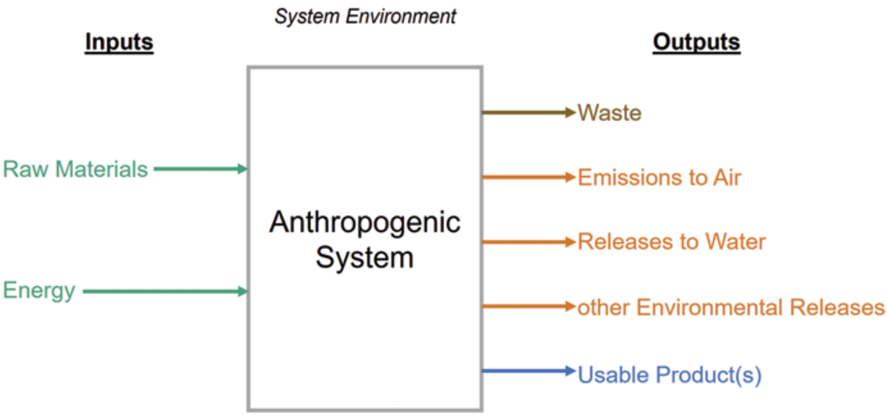

Fig. 2.2 Basic model of life cycle inventory modeling: an anthropogenic system with interventions to the environment, distinguished in different types of flows. (Fava et al. 1991, adapted)

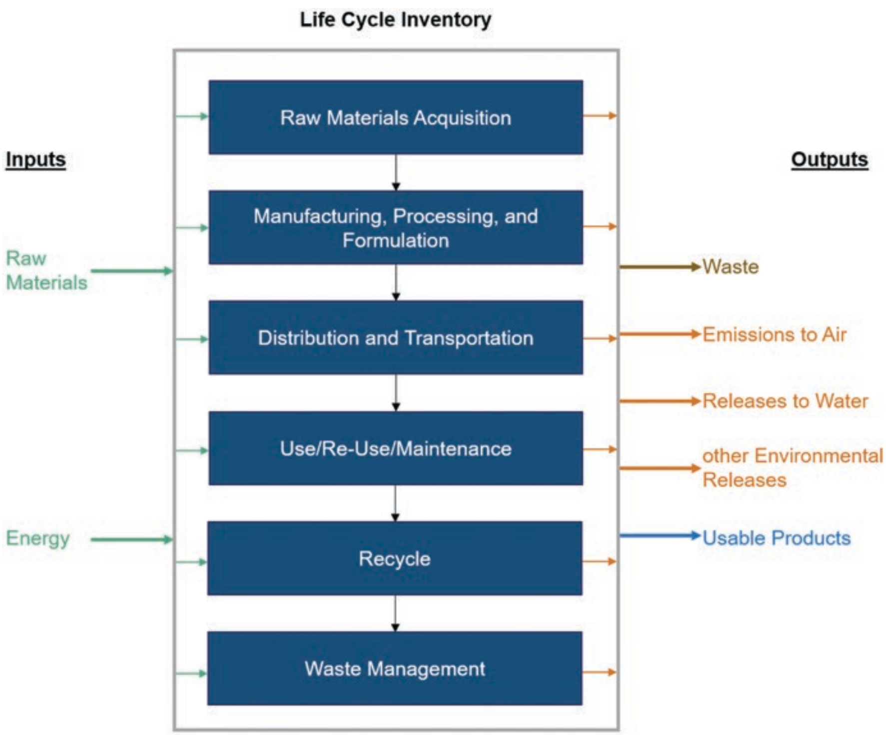

Fig. 2.3 Life cycle stages in an LCI model. (Adapted from Fava et al. 1991)

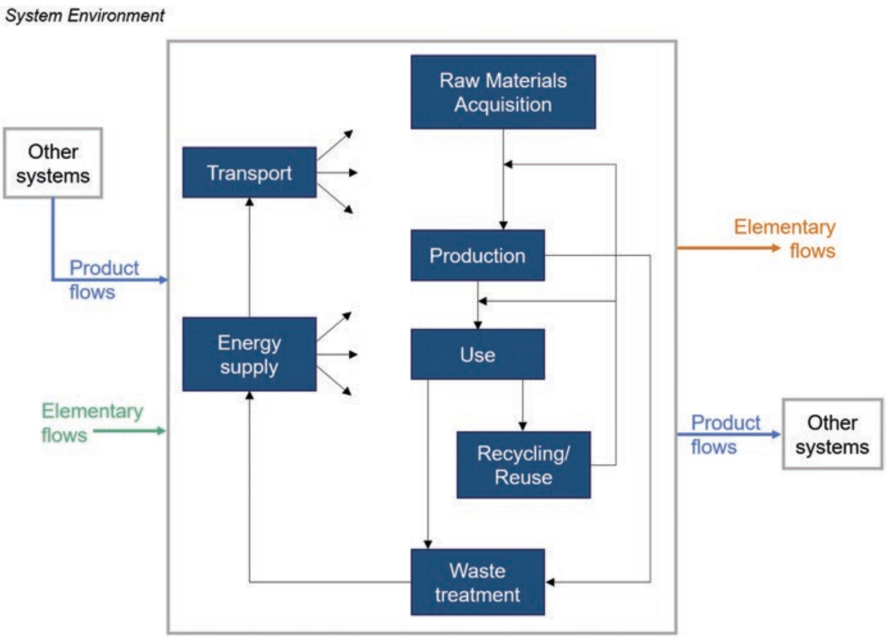

Fig. 2.4 A schematic life cycle with example processes (ISO 2006a): some flows (e.g., from transport and energy processes) can be used several times, while others can create loops within the analyzed system (e.g., flows from recycling)

inputs from other product systems in the form of products. Figure 2.5 shows parts of a more realistic case.

This bundle of connected processes is also called a *product system*. It is delivering the functional unit of an LCA case study. Each process is called *unit process* and it is typically modeled as a black box (Fig. 2.6), with a fixed relation between inputs and outputs. This means that all inputs and outputs linearly depend on the amount of the product needed (i.e., *usable product* in Fig. 2.6): if two units of product are needed instead of one, all flow amounts in the process are multiplied by a factor of two. The whole product system model in an LCA is therefore a relatively simple, but large, linear model.

For a given process, not all flow types may be present. As an example, Fig. 2.7 shows the data set of the process of soy biodiesel production from LCA Commons (https://www.lcacommons.gov/), with several input products, water as input resource, two output products (glycerin and soy biodiesel), and fatty acids as emissions into water.

This linear model, which describes processes as input/output "boxes" connected by exchanging products and distinguished into several life cycle stages, is **the basic LCI model**. As mentioned, this model is a simplification of reality in several aspects. This makes sense, since the task, to model the impacts caused by a product over its entire life cycle, is complex and demanding. In reality, life cycles are infinite

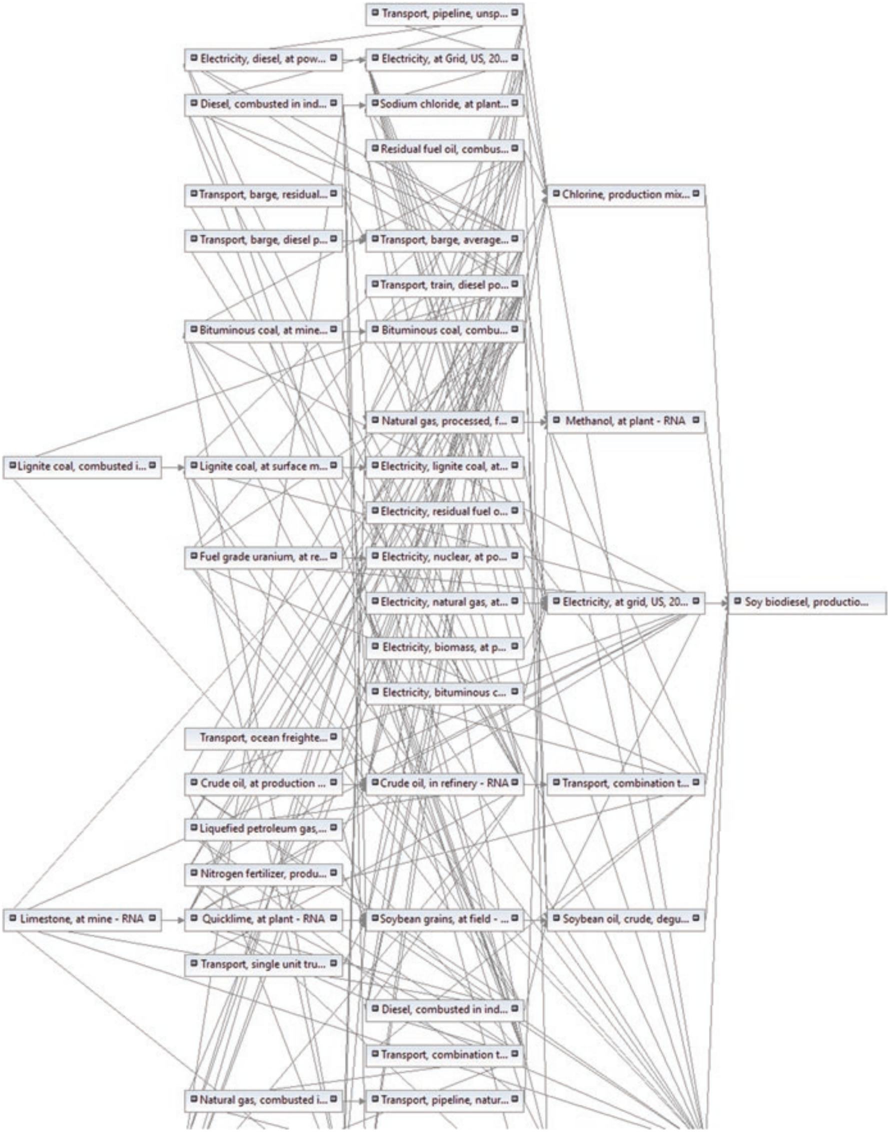

Fig. 2.5 Parts of a realistic life cycle for soy biodiesel production. Screenshot from openLCA using processes (represented through boxes) from LCA Commons (https://www.lcacommons.gov/)

and for many processes, the input amounts do not depend linearly on the product produced (e.g., for agricultural processes, Heady 1958), the scale of the process has an influence on process inputs and outputs, especially for industrial processes (Encyclopaedia Britannica 2011; Piccinno et al. 2016), and impacts vary over time and space. Therefore, the basic LCI model is simple, robust, and relatively easy to

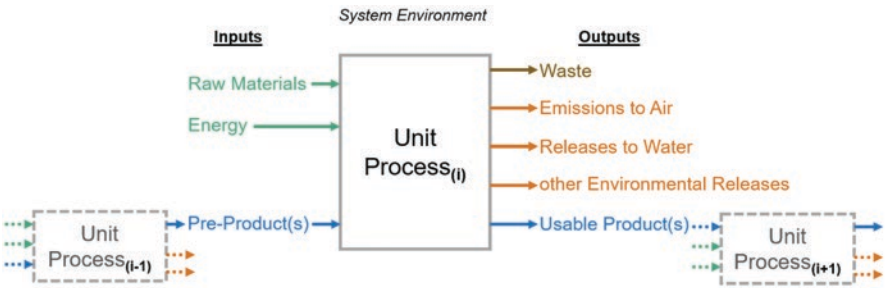

Fig. 2.6 Principal structure of a unit process data set, with energy, raw materials, and pre-products on the input side, and emissions to water, air, and other environmental compartments, as well as waste and products

Inputs				
Flow	**Category**	**Flow property**	**Unit**	**Amount**
Citric Acid, at plant		Mass	kg	0.00245
Hydrochloric Acid, at plant		Mass	kg	0.146
Phosphoric Acid, at plant		Mass	kg	0.00213
Sodium Methylate, at plant		Mass	kg	0.0777
Electricity, at grid, US, 2000	Utilities/Electric Power Distribution	Energy	kWh	0.12
Methanol, at plant	Chemical Manufacturing/All Other Basic Organic Chemical Manufacturing	Mass	kg	0.305
Natural gas, combusted in industrial boiler	Utilities/Steam and Air-Conditioning Supply	Volume	m3	0.0762
Sodium hydroxide, production mix, at plant	Chemical Manufacturing/All Other Basic Inorganic Chemical Manufacturing	Mass	kg	0.00327
Soybean oil, crude, degummed, at plant	Chemical Manufacturing/All Other Basic Organic Chemical Manufacturing	Mass	kg	3.32
Transport, combination truck, diesel powered	Truck Transportation/General Freight Trucking	Goods transport (mass*distance)	t*km	1.24
Water	resource/unspecified	Volume	l	1.14
Outputs				
Flow	**Category**	**Flow property**	**Unit**	**Amount**
Fatty acids	water/unspecified	Mass	kg	0.00694
Glycerin, at biodiesel plant	Biofuels Manufacturing/Biodiesel	Mass	kg	0.403
Soy biodiesel, production, at plant	Biofuels Manufacturing/Biodiesel	Mass	kg	3.36

Fig. 2.7 Snapshot of soy biodiesel production dataset from the LCA Commons database (https://www.lcacommons.gov/)

compute, but it presents some key modeling aspects, as well as some possibilities for extensions. In the following Sects. 2 and 3, these modeling aspects and extensions, respectively, will be described together with a number of examples. In Sect. 4, some conventions for modeling transport services, the use phase, and the end of life in LCA are presented.

2 Some Fundamental Modeling Topics in the Basic LCI Model

Some aspects are fundamental to modeling the life cycle, following the idea of a basic LCI model: modeling the benefit a product provides, setting the system boundaries, and modeling what is caused by consuming a product, that is, which other production processes are triggered if product of one specific process is consumed. Further, the location of emissions and of the activity itself, and not the least the question of when a process can be considered as being complete. These aspects are further explored in the following.

2.1 Modeling Benefits and Impacts: The Functional Unit

Already in the very early days of LCA, the emphasis was put on how to develop an inventory model (and LCA) that is suited for a fair comparison of different products. The basic idea of enabling a fair comparison is based on benefits and impacts related to a product: Every product has more or less negative impacts (emissions to the environment and resource use); on the other hand, every product brings benefits to its user, and these benefits are the reason why the product is produced and then consumed. To allow for a fair comparison of different products, it must therefore be ensured that the products to be compared provide the same benefit. If this is the case, the product with the least environmental impact is preferable. This is shown in Fig. 2.8 for a theoretical case, with three different products having different benefits and impacts. Since product 1 and product 3 bring the same benefits, it is possible to say that product 1 is better than 3 since it causes lower impacts. However, since benefits differ between product 2 and product 3, which of these is preferable is unknown – product 2 has lower impacts but also less benefits, while product 3 has more benefits but also higher impacts.

The product's benefit is represented by the *functional unit*, which is defined in ISO 14040 as "quantified performance of a product system for use as a reference unit" (ISO 2006a). The functional unit is directly linked to one specific or, more rarely, to different processes and their products via the *reference flow*, which is defined as a "*measure of the outputs from processes in a given product system required to fulfil the function expressed by the functional unit*" (ISO 2006a).

In the example of the soy biodiesel process shown in Fig. 2.5, the functional unit could be: *Production of 1 liter of diesel for use in common, unmodified diesel engines, in mixture with fossil diesel, cetane number to measure ignition speed of 51* (Knothe 2006). The reference flow would be 1 liter of soy biodiesel according to the specification provided in the functional unit. With this functional unit, the soy biodiesel process and the preceding/upstream life cycle can be compared to a

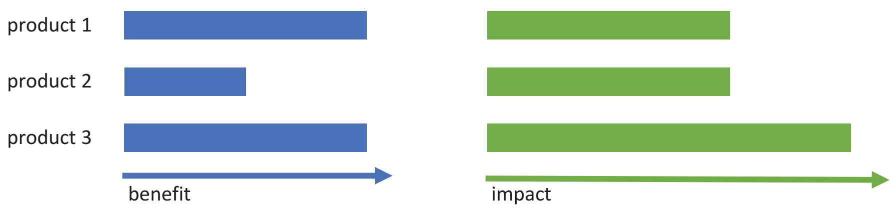

Fig. 2.8 Products 1, 2, and 3; product 2 offers less benefit than products 1 and 3, but similar or higher impact. Among products 1 and 3, product 1 has the lowest impacts and is therefore preferable

conventional diesel generated from fossil sources, with the same functional unit and an equivalent reference flow. Defining the functional unit is crucial for the outcome of a product comparison (e.g., Ciroth and Srocka (2008)), and is often discussed in LCI modeling and review. Common functional units are units of mass (1 kg or ton), volume (1 liter or m^3), energy (1 MJ or kWh), and 1 item, but also 1 km of line of writing (e.g., to assess the performance of a pen), a specific performance in insulation expressed in terms of transmittance (e.g., in $Wm^{-2}\ K^{-1}$ to assess insulation panels).

The functional unit is defined in the goal and scope phase of an LCA and represents the starting point of an inventory model (Curran 2017). This latter starts with questions as of how, meaning via which processes, the functional unit is provided or can be provided. The definition of functional unit in the goal and scope definition phase makes the inventory modeling focusing only on negative impacts related to input and output flows of processes. Only in cases of avoided or consumed emissions, and avoided resource use, can positive impacts occur. The rather unusual cases where a product has direct environmental benefit, not only indirectly via avoided emissions, are seldom considered. As examples, off-shore wind energy parks are said to have positive impacts on marine wildlife, once installed (Slavik et al. 2018); in social LCA, which generally claims to follow LCI modeling, some impacts can be positive, such as the creation of knowledge-intensive jobs and contribution to local development (Di Cesare et al. 2018). Such positive impacts are commonly not included when defining the functional unit.

2.2 *Modeling Causality: Attributional Versus Consequential Perspectives*

As explained in the previous section, an LCI model refers to the consumption of a certain amount of a given product, which is specified by the functional unit and the reference flow. The entire LCI model can then be seen as an answer to the question: Which production processes are triggered by the consumption, in the given amount, for the specified product? The answer to this question is decisive for the development of the entire model. It not only needs an answer for the final process, which is providing the product of the functional unit, but for any other product that is appearing as input in the included processes as well. In LCA, two principally different approaches for answering this question have evolved, called attributional and consequential LCA modeling. The corresponding LCA models are quite different, for example, regarding system boundaries, required input data, and allocation (Ekvall et al. 2016) (Table 2.1).

Attributional LCA was originally proposed by Heijungs (1997) with the aim of providing information on the portion of "global burden" associated with a product and its life cycle. This approach is based on the ceteris paribus assumption, meaning that the choice of the functional unit (i.e., linked to a certain amount of product)

Table 2.1 Characteristics of accounting type and change-oriented LCI models (Tillman 2000)

Characteristics	Type of LCA	
	Accounting (attributional)	Change-oriented (consequential)
System boundaries	Additivity	Part of system affected
	Completeness	
Allocation procedure	Reflecting causes of system	Reflecting effects of change
	Partitioning	System enlargement
Choice of data	Average	Marginal (at least in part)

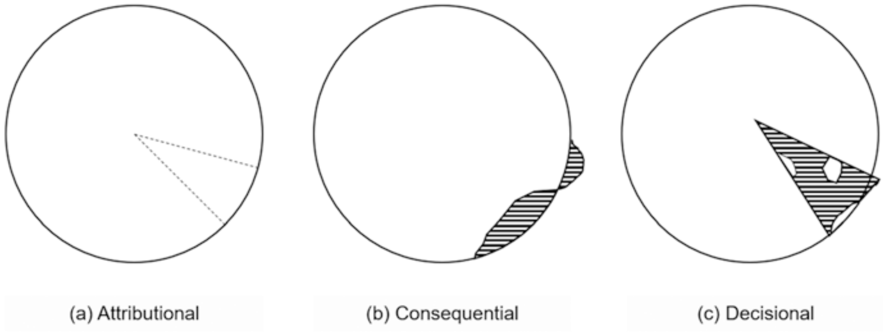

Fig. 2.9 Attributional, consequential, and decisional LCA (adapted from Weidema 2003). The entire pie represents the whole production (or market) of a product, the slice represents the functional unit analyzed in a study and the dashed areas represent the portion of the market influenced by a decision

does not influence the other activities on the planet, including the overall production and consumption of the product under study (Heijungs et al. 1992; Frischknecht 1998; Ciroth and Srocka 2008). Therefore, the functional unit can be directly linked to the overall product production, with its inputs and outputs occurring within a certain time (Curran et al. 2005), through the reference flow (i.e., amount of product required in the functional unit). Referring to Fig. 2.9a, an attributional LCA can be visualized as a slice of the whole product pie, where the functional unit defines how large the slice is.

Regarding the model, attributional LCA fits well with a linear modeling approach. If attributional LCAs of all final products were conducted, the total environmental burdens worldwide would be estimated. According to the superposition principle of linear systems, the impact of a larger system results from the sum of impacts of all single sub-systems. In addition, the resulting impacts are linearly proportional to the assumed produced quantity, and all inputs and outputs are equally allocated to each single unit of the reference product (e.g., each kg). Such an attributional analysis of a product usually considers current average market conditions.

Despite attributional LCA probably being the historically most common approach, *consequential LCA* has been gaining popularity in the last decade (McManus and Taylor 2015). Consequential modeling aims at modeling direct and indirect changes in the production system and system environment induced by decisions, or in short, consequences of decisions (Ekvall and Weidema 2004). The consequential modeling approach was proposed with the idea that attributional LCA is for certain markets not able to adequately reflect real impacts: If markets are constrained so that additional product consumption cannot be realized by increased average production, attributing the average production to new consumption is not a good estimate. In that case, no additional consumption can take place and, typically via higher prices, an increased competition for the existing products occurs, where previous consumption is discontinued. Alternatively, the market is expanded by installing new production capacity, which might be different from the market average production. These decisions can regard investments in new products or modifications of existing production processes, and can lead to changes in the market and consumption patterns, such as technology switches, changes in the market share and learning curves (Curran et al. 2005). Consequential LCA thus describes environmentally-relevant physical flows to and from a life cycle and its sub-systems that are influenced by a decision (Ekvall and Weidema 2004). These environmentally relevant consequences depend on:

1. The consumed amount of the product under study, or preferably the increased or decreased demand for the product. These changes can be short term (e.g., changes in output from existing production capacity) or long term, which regard changes in the timing, and perhaps the nature, of investments in new production capacity (Curran et al. 2005).
2. How constrained the market of this product is regarding whether additional consumption can be satisfied with the existing production capacity. Therefore, consequential modeling generally assumes that the required additional production capacity is satisfied through alternative, usually newer, technology, compared to the market average.

Referring to Fig. 2.9b, a consequential LCA can be visualized as a change to the overall product pie. The operating assumption behind consequential LCA is that a particular decision regarding a production process affects other production processes (e.g., changes in their outputs) due to cause-effect chain relationships. Specifically, the consequential approach aims to link microeconomic actions with macroeconomic consequences (Frischknecht and Stucki 2010), and it is argued to be suitable to evaluate the environmental consequences of decisions (Tillman 2000), especially of "big decisions" (Brandão et al. 2014). For this reason, the rules used to define which processes are included in or excluded from the product system are based on estimations of how material and energy flows will change due to the analyzed potential decisions, meaning that a consequential LCA study only includes processes that are affected by this decision (Curran et al. 2005). Consequently, consequential LCI models describe supply chains embedded in a dynamic technosphere that reacts to changes in the demand for different products (Sonnemann et al. 2013). Therefore, consequential LCIs could include alternative use of constrained production factors (i.e., constrained market), general market effects, identification of the competing products, identification of marginal technology, and technology development (Ekvall and Weidema 2004).

LCI models are in principle steady-state, linear, and homogeneous, with each unit process fixed at a specific point in time (Suh and Huppes 2005; Consequential-LCA 2015). But in consequential modeling, the decision depends on the specific product analyzed and amounts affected, as well as on available technologies on the market, which involves several competing alternative technologies, making the system modeling more complex. For this reason, consequential LCI models can, for example, involve partial or general economic equilibrium models to describe market reactions (Ibenholt 2002), agent-based models to include human behavior and local variabilities (Baustert and Benetto 2017), or dynamic models to build one or several scenarios to be used as (per-defined) conditions (Frischknecht and Stucki 2010). Despite consequential models are claimed to describe how activities influence each other and their environment (Weidema 2016) and thus not to be scenario modeling, they often include scenarios to describe alternative decisions (e.g., Yang 2016). While theoretically convincing, it is often difficult to model consequences in a clear and unambiguous way: Even if consequences are defined for the specific case study, a specific new technology introduced in the market can substitute several existing ones.

A third approach, called *decisional* or decision-oriented LCA (Fig 2.9c), represents an alternative definition of the consequential approach focusing on the microeconomic level (Frischknecht 1998). The main basis of information for constructing the product system in the LCI are actual or anticipated financial and contractual relations between economic actors (business-to-business relations). Consequently, the economic and/or contractual links define which processes are included or not in the LCI model (Frischknecht and Stucki 2010). Decisional LCA aims at supporting decisions in companies to improve the environmental performance of their products or processes.

This section represents a brief summary of the different LCI modeling approaches. Given the huge amount of existing literature and the ongoing debate, the presentation and discussion on the different LCI modeling approaches would have deserved a full dedicated chapter. Nevertheless, the reader can access the cited literature to dig deeper into the topic.

2.3 Setting Boundaries in an Infinite Inventory Model

Setting boundaries is one of the crucial steps in LCA and LCI modeling, since it prevents, ideally, the following of supply chains that are not contributing considerably to the overall result, and thus helps to focus on the important parts. An explicit specification of system boundary setting is fundamental also for carrying out fair comparisons of products. Issues related to setting the boundaries are present both within the technosphere as well as between the technosphere and the biosphere. Within the technosphere, any life cycle is in principle infinite (Baumann and Tillman

2004): for instance, referring to the soy biodiesel production in the US (see Fig. 2.5), it may need Japanese machines, which in turn need electricity from the Japanese electricity grid mix, which again needs, for the nuclear power share, uranium from Kazakhstan, which again is produced using machines from Russia, and so on. In order to deal with boundaries within the technosphere, two approaches are common.

Firstly, quantitative cut-off rules are applied to define the technosphere's boundaries and the related data collection. In a well-specified system, amounts of flows, scaled to the functional unit and reference flow, will become smaller and smaller while going backward in the supply chain. Also, loops in the system, created by a process delivering its inputs as outputs, directly or via other processes, will converge. For example, steel production will require some steel, but not more steel than the steel production produces. Similarly, corn production will require a certain amount of corn to be used as seed, but less than the corn that is produced, otherwise the entire production process does not make sense. Quantitative cut-off rules specify a threshold; products that do not provide, scaled to the quantitative reference flow, a certain quantitative amount above the threshold are not included in the system, nor their upstream supply chain. With amounts becoming smaller and smaller for processes that are "more remote" from the process delivering the functional unit, a threshold thus delimits the size of the overall investigated system (Fig. 2.10).

The threshold amount is typically defined based on the amount of the product in terms of energy or material. If products have different units (e.g., a liter of diesel vs kg of soybean, or a piece of a car vs amount of metal sheets in kg), the quantitative cut-off may not be able to fully reflect the quantitative contribution of the flows to the overall inventory result.

Secondly, each flow amount is only a proxy of the contribution to the environmental impacts. Therefore, the ISO 14040 standard mentions that cut-off thresholds can also be specified in terms of (relative contribution to the) environmental impacts (ISO 2006a). However, when building a product system and when deciding whether to include a new process or not, the entire environmental impact of the supply chain

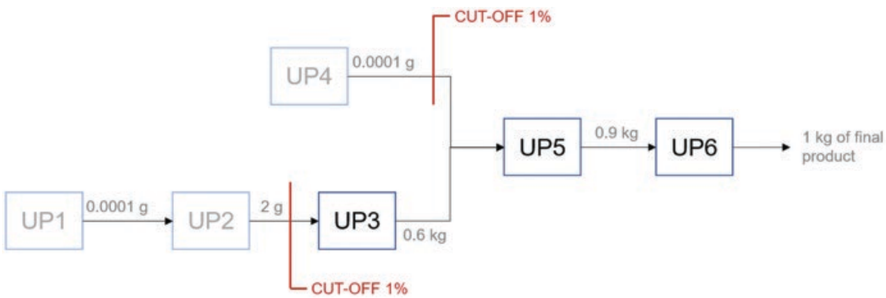

Fig. 2.10 The application of cut-off excludes the processes and the flows that contribute less than the fixed cut-off threshold. In the picture, the cut-off is set at 1% and all the flows below this threshold, that is, below 10 g, are excluded from the LCI model. (UP = unit process)

of that process are not known, and thus the environmental impact cannot really be considered as a threshold.

A third type of cut-off rules exclude processes or flows that fall into a certain type or classification, typically infrastructure. This "discriminating cut-off" is justified by analysis that under certain conditions, infrastructure does typically not contribute to the result of an LCA considerably (Frischknecht et al. 2007).

Fourthly, an LCA study can focus on some specific steps in the life cycle only, cutting off the others. Common cases are the cradle to gate studies, comprising the life cycle until the product leaves the producer, thus excluding use and end of life phase. This is, however, not typically considered as a cut-off, and will not be discussed further here.

Cut-off criteria discussed so far are applied when building the life cycle inventory. Their use must be specified in the goal and scope definition phase of the LCA. While being helpful for creating models and focusing the effort on the parts in the life cycle that matter, they are only supported directly by few LCA software systems, suffer from different units in databases,[1] and only approximating the actual impact to be assessed.

Another use of the cut-off criterion is ex post, for quality assurance of already created systems. Several Environmental Product Declarations, and also the Environmental Footprint Category Rules, specify that overall the amount of excluded materials must not exceed a threshold, or also that the excluded environmental impact must not exceed a certain threshold (e.g., European Commission 2018). In these cases, the threshold exceedance can only be calculated once the full, infinite but converging, system is known.

In the best case, no threshold and cut-off are applied. According to ISO 14040, "[t]he system boundary defines the unit processes to be included in the system. Ideally, the product system should be modeled in such a manner that inputs and outputs at its boundary are elementary flows…" Setting boundaries between the technosphere and the biosphere, that is, defining which are technical and elementary flows, is not always trivial. Potentially, this boundary can be precisely defined for nonrenewable resources (e.g., where a metal is extracted from a mine), while it is more difficult for renewable ones, both for found (e.g., forests and agricultural land) and flowing resources (e.g., solar radiation) (Baumann and Tillman 2004). Similarly, it is not always easy to define whether agricultural soils are part of the technosphere or the biosphere. Soils are essential components of technical activities such as plowing, tillage, mechanized planting, and harvesting, as well as fertilization and pest control. Nevertheless, soils have important ecological functions through which they provide the so-called supporting ecosystem services, which are part of the biosphere (MEA 2005). The definition of system boundaries in agricultural production systems is important and has a great influence of the results (Roer et al. 2012). This definition is further affected by complex soil dynamics (e.g., soil erosion, nutrient

[1] Which means, on the other hand, that they are more powerful in databases such as input-output databases where all product flows have the same unit.

leaching, nitrous oxide emissions) (Li et al. 2007), which are difficult to control. For example, regarding climate change, carbon net sequestration or emissions only occur when the soil management type has been changed until a new equilibrium level of carbon in the soil is reached (Tuomisto et al. 2012); additionally, the status of carbon in the soil and carbon flows also depend on the history and on the location of the soil under study.

The definition of boundaries between the technosphere and the biosphere regards also the "grave" side of the product life cycle. In particular, this applies to the case of landfill sites and the related long-term emissions, which are introduced in Sect. 3.2. Two main approaches have been proposed in the literature to address this kind of temporal boundaries (Baumann and Tillman 2004): (i) gathering emissions data within a certain period to complement the inventory, and accounting for the remaining materials after that period in a separate data category (Tillman et al. 1994), or (ii) including the landfill in the inventory until all the material is degraded (Finnveden et al. 1995).

To conclude, the system boundary is specified in the goal and scope definition of an LCA, as also explained in the ISO (2006a) and Curran (2017), but in this section, we have seen that it has several feasibility implications in the LCI modeling, which are still under debate.

2.4 Modeling Locations

Modeling locations in LCI models are interesting for a variety of reasons, both in the definition of the product system, in the LCI model, and in the impact assessment. Firstly, to build a realistic model, the location of a process delivering a product and the location of the process receiving that product needs to be identical, if the two processes are not linked with a transportation service: for instance, electricity from Norway cannot directly be used in Germany; it needs to be transported first. Secondly, processes and related flows can differ in different locations, especially when they depend on nature. For example, the same agricultural process might need a different amount of (or no) water at all in different regions due to different climatic conditions. Similarly, a photovoltaic cell will have different yields per year, depending on the altitude and the latitude. Thirdly, the same withdrawal of resources or release of emissions may have different impacts depending on the location, for example, on the availability of resources in the location or the status of air or water bodies. Emitting particulate matter has higher impacts in inner cities where more humans are exposed and withdrawing water in the arid region such as the Arabic peninsula has higher impacts than withdrawing the same amount in water-rich areas, such as the Netherlands. The required spatial detail and resolution depends on the scale of impacts, that is, if they are local, regional, or global.

To model locations in LCI, there is currently not one single, agreed-upon approach. Depending on the LCA databases and tools, different approaches are instead applied. As a basic approach to address locations, most LCI databases further classify flows into sub-compartments (e.g., the ecoinvent and the ILCD/PEF database). This allows for specifying (i) if emissions into air occur in high-population or low-population density area, which is useful to improve the characterization of human health-related flows; and (ii) if emissions into soils are located in agricultural, industrial, or forestry areas, or if water emissions end up into different types of water bodies (lake, groundwater, river, fossil water). This approach can be referred to as spatial archetypes (Mutel et al. 2018).

In addition, flows can be also regionalized or countrified, meaning that the database provides individual elementary flows for specific countries or regions, which are usually characterized using an ISO two-to-three letter code, possibly adapted and extended by different available databases (e.g., RER = rest of Europe, CH=China and RNA = rest of North America in ecoinvent). This approach can be adopted for and applied to processes. With this approach, flows can obviously be distinguished by country, and thus water withdrawal in Saudi Arabia can be distinguished from water withdrawal in the Netherlands. A drawback is that each flow is repeated for several locations and the dimensions of the database increase.

In the ILCD format, the flow is therefore not linked to a location, but instead only the exchange (i.e., the link between a flow and a process), meaning the flow, when it is input or output of a process, is linked to a location (Fig. 2.11).

This does not increase the number of flows in a database but is at present not yet supported by LCA software tools. Furthermore, a country or region, characterized with an ISO code, is not fully homogenous. Knowing that a given water withdrawal takes place in big countries, such as Russia, the US, and China, does not help much to understand the impact. Some LCA software systems integrate geographic information system (GIS) data or provide interfaces to GIS (at present, openLCA and brightway2). The use of GIS files makes the selection of the location more flexible. This improves the impact assessment, especially for those environmental impact categories focusing on the local scale, for which the country scale is too coarse. Those potentially more accurate inventories should be coupled with impact assessment methods able to deal with the same spatial scale (Frischknecht et al. 2018). For instance, when dealing with water, the water basin or watershed scale is usually adopted. For the AWARE water footprint method, a flow-based regionalization method with country-specific characterization factors for water scarcity is available, which is for big countries such as China typically not indicating the impact of water withdrawal at one given site (Boulay et al. 2018). In China, the water availability highly varies throughout the territories: The national average is about 43 m^3/m^3, meaning that China has about 43 times less available water remaining per area than

Fig. 2.11 Process, exchange, flow, and location, in the ILCD format

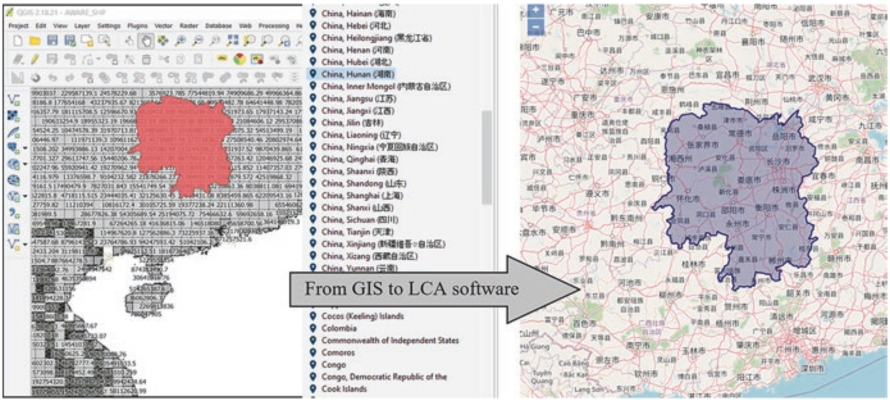

Fig. 2.12 Integration of GIS software (Q-GIS) and an LCA software (openLCA) to perform the geospatial-based regionalization. The left-side figure shows the south-eastern part of China (in gray) and the Hunan region highlighted in red; the grid shows information about water availability (from WaterGAp model, Flörke et al. 2013; Müller Schmied et al. 2014) in each single cell. The right-side figure shows the openLCA interface showing the same location (with OpenStreetMap, https://www.openstreetmap.org/, in the background)

the world average. This means that, if 0.5 m^3 water is used in China, the resulting impact will be about 22 m^3 (i.e., about 43 times higher than the input value). But China also has rainy regions, like Hunan (Fig. 2.12), where the average annual precipitation ranges between 1500 and 2000 millimeters (Hunan Gov. 2018). By integrating georeferenced watershed level characterization factors provided by the AWARE method and calculating the characterization factors specific for the Hunan province, a value of about 0.4 m^3/m^3 is instead obtained, and the impacts caused by the use of 0.5 m^3 of water instead becomes 0.2 m^3, about 100 times lower than the previous estimation.

With GIS integration or interfaces, there is no limit to the timely resolution of the inventory and of the impact assessment models, but it is evident that this can lead to extremely large models. As often in modeling, there are trade-offs between model sophistication and accuracy and effort spent.

Typically, in most LCA studies, specific geographical locations will be modeled for the foreground system only, while for the background system, generic locations might suffice, as they are provided in databases. These generic locations, however, can also be modeled following a site-specific approach, in case of large water power plants for example (Ribeiro and Anderi da Silva 2010).

In summary, modeling geographical location in LCA is still under development and the comparability and reproducibility of regionalized LCAs are not facilitated by any standards yet (Frischknecht et al. 2018). Nevertheless, the opportunities for the near future seem promising especially given the great availability of spatially explicit information available.

2.5 When Can a Process Dataset be Considered Complete?

As introduced in Chap. 1, an LCA tries to provide a comprehensive view of the environmental impact related to a product or service, in line with a specified goal and scope; the smallest modeling entity of a life cycle inventory model are process datasets. This directly raises the question as to when a process dataset can be considered complete. The requirement to provide complete or almost complete datasets can be found in almost all recent data quality management systems in LCA, see Chap. 5. So, under which conditions can a dataset be considered "complete"? There are three aspects to consider.

Firstly, the goal and scope specified for the dataset, the entire database, or also for the study determine the intended use and the impact categories and impact methods a dataset is supposed to support. For example, in one of the very early LCA studies, ozone depletion could not be considered as category, since in the data collection, ozone-depleting substances were not covered: *"the present LCI results do not allow for a consideration of the category Ozone Depletion, since in data collection, ozone depleting substances […] were disregarded"* (Schmitz 1995, p A12).[2] In addition to the supported LCIA methods, goal and scope also specified the nomenclature and thereby the structure and detail for the flows, to, for example, understand whether a dust emission should be called "dust," "fine dust," "particles," or be distinguished into "PM10," "PM5," and "PM2.5," to name just some examples.

Second, completeness is to be assessed based on the set of flows provided for the dataset; does it include, for example, CFC emissions, if these are present, or have they been skipped? Ideally, the dataset contains all flows occurring in reality, following the specified nomenclature.

Third, a dataset should have an even mass and energy balance, given that the basic LCI model does not foresee any stocks to be "stored" in the dataset: all masses that enter the process need also leave the process.

While it is easy to spot usage of inappropriate nomenclature in a dataset, it is much more difficult to see whether all resource needs and emissions have been listed, and even more whether the amounts are fitting to the real process.

3 Extensions of the Basic LCI Model

3.1 Modeling Multifunctionality

In the simplest case, each process produces one product, which represents the purpose or function of the process, meaning that the process is happening because there is demand for this product (e.g., a photovoltaic cell is built and installed because electricity is required). This latter links this process to other processes in the product

[2] Translated to English by the authors

system, making it the final product (i.e., quantitative reference) of the product system under study. Quite often, however, a process is creating more than one product (Fig. 2.13), and thus has several functions. For instance, in the soy biodiesel process shown in Fig. 2.5, there are two products: the main product soy biodiesel and the byproduct glycerin.

How can inventory models deal with such multifunctionality? This is one of the "classic" questions in LCI modeling (Russell et al. 2005). The ISO recommends a stepwise procedure (ISO 2006b). Firstly, to avoid allocation:

1. Dividing each unit process into subprocesses (each one referred to one coproduct) and gathering the additionally required environmental burden data.
2. Expanding the product system boundaries to include additional functions related to the coproducts.

If these options are not possible, then allocation is recommended:

3. Distributing ("allocating") the environmental burdens of each product based on their underlying physical relationships, i.e. their mass, or energy content for example.
4. If allocation based on physical relationships cannot be done, then this allocation of the environmental burdens of each product needs to be done based on other rules; often, economic relationships, i.e. the price of the products, is then used.

When developing an LCI model, the three approaches reported in the ISO standard have a different practical implementation. In the first case, system subdivision, additional effort is required to refine data collection while focusing only on the product under study, which in real systems is often not feasible (Fig. 2.14). Additionally, to have accurate information and results, the subprocesses should be physically and economically independent (Ekvall and Finnveden 2001). In the end, subdivision is possible in cases where the two independent processes have been lumped together somewhat thoughtlessly in an initial model. An example: A soybean farmer may produce soybeans and also wheat, but for 1 year in different fields; for an LCI model, a combined process could be created that produces both wheat and soybeans, and thus is a multifunctional process. Instead, though, two processes

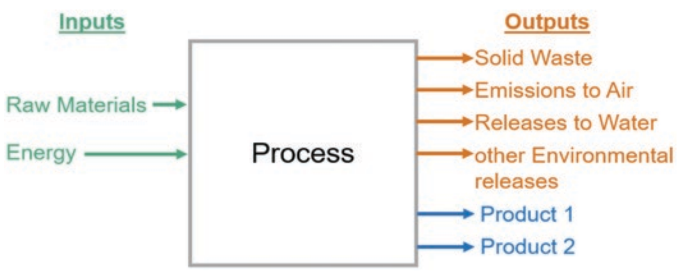

Fig. 2.13 Production system producing two usable output products

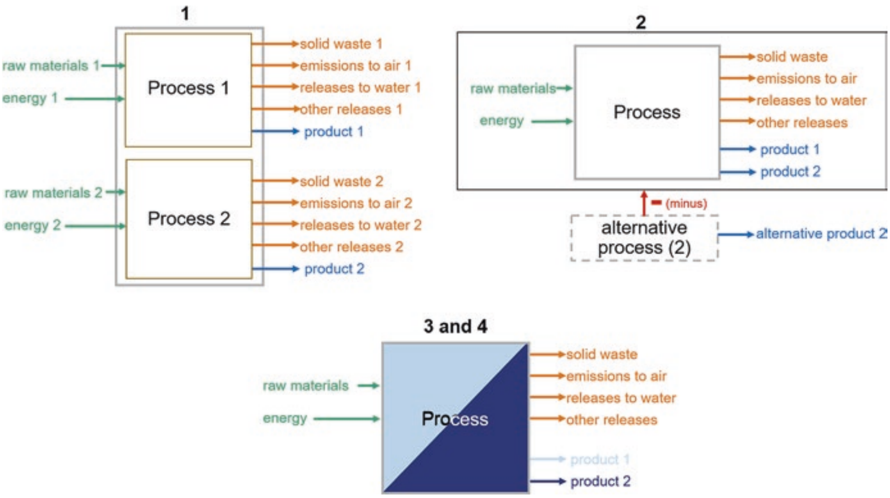

Fig. 2.14 Dealing with multifunctionality: system subdivision (1), system expansion (2), avoided burden approach), and allocation (3 and 4)

could be created as well, the one producing wheat, the other soybean, without the need to apply allocation or system expansion.

Secondly, system expansion can be performed via system enlargement or the avoided burden approach (Azapagic and Clift 1999), which consists of either adding or subtracting (Fig. 2.14) the environmental burden of an *alternative production process* (Reap et al. 2008). The alternative process provides then only the one byproduct from the initial process, and its purpose is to basically get rid of the byproduct. Including alternative production into the LCA model is not always an easy task since it leads to a larger, more complicated model that requires more data (Curran et al. 2005). Additionally, (i) an alternative process may not exist, or (ii) there may exist more than one alternative process, and (iii) the required inventory for the alternative process may not be accessible or reliable (Azapagic and Clift 1999).

Thirdly, the allocation is an option (Fig. 2.14); it is sometimes considered as one of the most controversial issues in LCA (Rebitzer et al. 2004; Reap et al. 2008). As previously said, different allocation rules exist (e.g., physical or economic), and it typically cannot be stated that one single method of these is best or provides a generally acceptable solution (Curran 2007). Dealing with multifunctionality thus remains a matter of choice in the approach and in the method within each approach. The decision for one or the other way to deal with multifunctionality should be made in the goal and scope definition since it might have a strong implication on the created LCI. For a deeper discussion about the multifunctionality problem, see Chap. 4.

3.2 Modeling Time

Real-life production processes, and consequently product life cycles, happen in and vary over time. Each single process in a life cycle is characterized by a certain temporal dimension (e.g., duration), for example, in the production steps and in the use phase. The LCI attempts to describe a dynamic, time-dependent, and successive-in-time technosphere, both in processes and supply-chains (Shimako 2017). However, the temporal dimension is normally not considered in the basic LCI model, which is rather agnostic about time. LCI is indeed implemented by assuming an "infinite" flow of products, from one process to the next one in a given life cycle, in consecutive periods of time (Fig. 2.15) and by assuming that all the involved technologies were to remain the same (i.e., steady-state technological relations between a process and its inputs and output flows) (Ciroth et al. 2008).

In practice, LCI results consist of absolute quantities (e.g., kg) and, despite their name, not of physical flows in a strict sense (i.e., kg year^{-1}). Emissions, consumed resources, and intermediate technological flows are expressed without a time indication. Nevertheless, time affects LCI modeling in a variety of ways. Here below, some examples are presented. Firstly, time affects different life cycle stages: (i) during the use phase, some products, such as vehicles and buildings, need maintenance activities. The models generally assume maintenance interventions at predefined time intervals over the (assumed) life span of the product; (iii) in real processes, a storage phase can occur between an input and an output, and in a

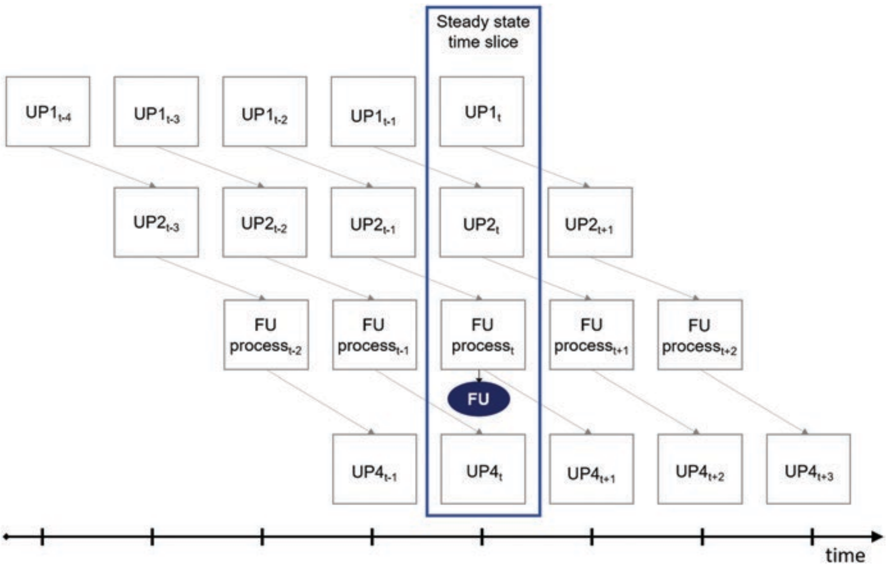

Fig. 2.15 Steady-state technological relations between a process and its inputs and output flows and steady state time slice analyzed with LCA (Adapted from Ciroth et al. 2008). (UP = Unit Process; FU = Functional Unit; t = unit of time)

warehouse, stock can decrease or increase. In balance sheet equations in engineering (e.g., Schütt et al. 1990), this effect is described with a storage term, while in LCI modeling this term is simply ignored. With this simplification, the input must always even output, and every flow must in principle represent a steady-state, where it is not possible to have ever-increasing or ever-decreasing stocks; (iii) products may last and be used for a very long time (e.g., buildings and infrastructures), so long that end-of-life options are hard to imagine, both in technological and regulatory terms.

Secondly, in seasonal processes, such as in agricultural systems (Notarnicola et al. 2017), input and output flows vary within a year and this is often not accounted for in LCA (Bessou et al. 2013). The consumption or acquisition of certain resources and emissions can have different impacts at different times and in different locations. For example, a certain amount of water consumed during the dry season has higher or at least different impacts than the same amount consumed in the wet season (Boulay et al. 2015a, b).

Thirdly, different technologies studied in LCA might have reached different technological maturity. In the early days of LCA, the objects of study were often products that were mature in the sense that they had been produced and used in society for a long time, such as steel, concrete, milk, and ketchup. Today, many of these mature products have been thoroughly assessed and the focus has often turned to the continuously ongoing technology development. New materials, products, and technologies are being researched and developed each day. The benefit of assessing technologies at such and an early stage of technological development is that much of their design is still open to alterations at modest costs and efforts. An example of an emerging technology could be an electric car, to be compared by the current mature personal transportation technology, which would be a car with a combustion engine. Such comparisons can be facilitated by envisioning the emerging technology in the future, more mature state, which might include both upscaled production processes and altered background systems (Hillman and Sanden 2008). This approach can be referred to as prospective or ex-ante LCA (Villares et al. 2017; Arvidsson et al. 2018; Cucurachi et al. 2018). There is yet no standardized method for estimating the future emissions and resource use related to an emerging technology. Rather, a number of different approaches are being tested. One approach is to apply scenarios reflecting future, large-scale production (Walser et al. 2011; Arvidsson and Molander 2017). Laboratory-scale production is typically characterized by low energy efficiency inefficient use of materials, such as solvents. At larger-scale production, on the contrary, saving energy and materials is of high environmental importance and might also bring benefits in terms of reduced costs. Another suggested approach is to apply technological learning curves for future upscaling in prospective LCI modeling (Bergesen and Suh 2016).

Additionally, within a life cycle, consumption of resources and emissions at different stages can occur at different times, sometimes with time lags of decades or even centuries. This time lag raises issues related to intergenerational fairness and equity-related to current and future impacts. Methodologically speaking, by assigning the same characterization factors to short-term and long-term emissions, the impact of the latter might be overestimated. Furthermore, "releasing a big amount of pollutant instantaneously generally does not have the same impact as releasing the same amount of pollutant at a small rate over several years" (Levasseur et al. 2010).

A simple time differentiation in common LCI has started at the beginning of 2000 (Hellweg and Frischknecht 2004), in particular, with a distinction between long-term and short-term emissions. In practical terms, the basic LCI model assumes the following (ecoinvent 2018):

– Short-term emissions (e.g., occurring with a time horizon of 100 years in the ecoinvent database) are included in the modeling and are all assumed to occur at the beginning of the analyzed horizon and therefore aggregated; long-term emissions (e.g., after 100 years) are usually disregarded; this is done to prevent distorting assumptions in case of continuous emission over very long time spans, which would lead to an infinitively high emission which could distort any inventory result in case of time neglect (e.g., the case of emissions from landfill sites, or Radon-222 emissions from Uranium extraction and milling).

A more complete temporal resolution over the entire LCI is also possible, as proposed in dynamic LCA (Levasseur et al. 2010). An inventory where temporal differences have been considered can be referred to as a temporally-differentiated life cycle inventory (Beloin-Saint-Pierre et al. 2017). Clearly, refining and increasing the accuracy of methods to describe flow dynamics would improve LCI modeling, but integration with impact assessment methods that consider this dynamic is needed. Nowadays, even if different methods have been proposed in the literature (especially in the case of climate change, see Brandão et al. 2013 for a review), the definition of characterization factors is based on annual averages, without really making a distinction of time horizons. The ecoinvent database, for instance, provides two options: (i) attributing the same characterization factors to both short-term and long-term emissions, leading to an over-estimation of the impacts; (ii) attributing no characterization factors to the long-term emission, leading to an under-estimation of the impacts.

Conceptually, though, integrating time in the inventory is not complicated. Processes need a start and an end time, and when building the life cycle, the software or practitioner needs to understand which processes start at which point in time. As a practical example for long-living goods, temporally differentiated inventory models and full case studies for train components were published around 2000 (Ciroth et al. 2003): in the inventory of a train component with a lifetime of 30 years, a series of processes happen, with daily cleaning of the train to refurbishment and predictive maintenance and occasional accidents, where some prevent the train from operating (Fig. 2.16).

Discounting methods have been developed specifically for LCI modeling to take into account the time effects of biogenic carbon emissions, meaning carbon-related input and output flows involving biomass. When biomass enters a production process (e.g., wooden furniture or building construction, or production of food), the resulting CO_2 can be considered as a negative emission in the LCI. Usually, when

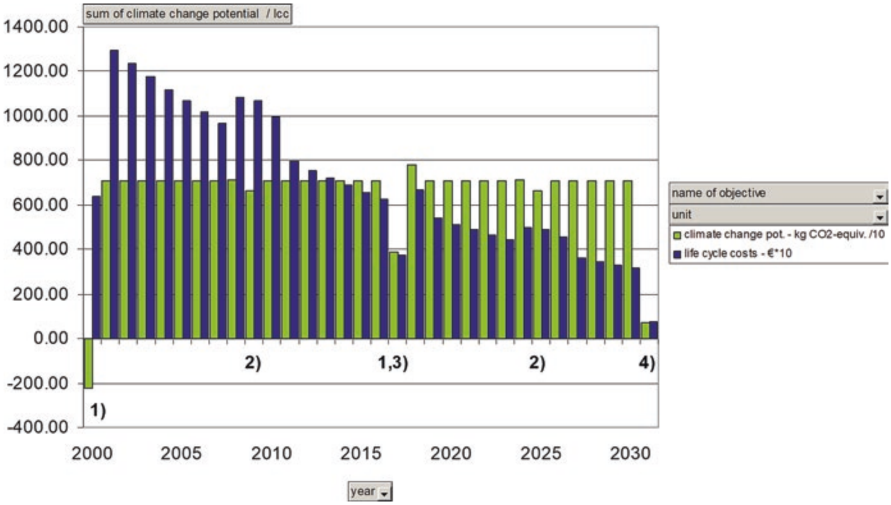

Fig. 2.16 Life cycle costing and climate change (in kg CO_2 eq) results for a wooden floor in a train carriage, operated for 30 years: (1) negative potential due to incorporated CO_2; (2) revision of the train; (3) modernization and reproduction of the floor; (4) disposal (waste incineration plant). Costs are discounted by 5% (Jensen and Remmen 2005, p. 84)

considering carbon uptake, a distinction is made between "short-living" goods, such as food, and long-living ones, such as furniture. The negative emissions of short-lived goods are typically not considered, since the CO_2 will be emitted again, for example, after the food is consumed, and a negative contribution to climate change for food at the point-of-sale might be misleading. For long-living goods, negative emissions are considered, since the goods "preserve" the captured CO_2. Altogether, different options in dealing with biogenic carbon uptake, storage and fixation, and removal are present in the literature:

– Biogenic carbon can be excluded from the inventory model entirely, that is, CO_2 fixation by vegetation is not considered, nor are downstream biogenic CO_2 emissions (e.g., in the case of food, or incineration of paper) (Milà i Canals 2007).
– Biogenic carbon can be considered together with the fossil carbon, that is, consider CO_2 fixation by vegetation as a negative emission and then account for the emission wherever it occurs (e.g., in waste treatment) (Milà i Canals 2007).
– Biogenic carbon can be distinguished from fossil carbon, and considered and reported separately from fossil CO_2, as required by the specific ISO for carbon footprint (ISO 2018).

Referring strictly to time, according to the ISO 14067 (ISO 2018), all the emissions (and removals) occurring over the life cycle "shall" be included without the effect of timing. This means that emissions arising from the pre-use stages, the use phase, and the end of life must be considered as single releases at the beginning of the time horizon chosen (Fig. 2.17).

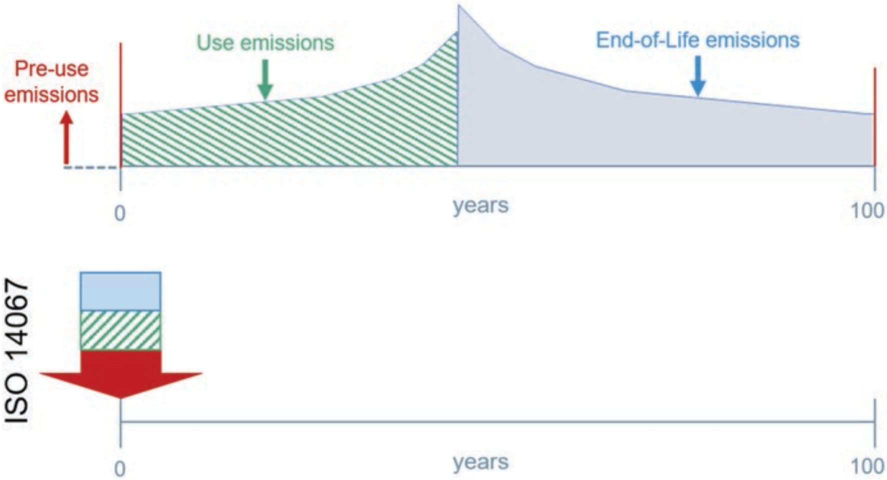

Fig. 2.17 Delayed greenhouse gas emissions: reality vs the ISO 14067 approach

The importance of considering the temporal dimension in LCA has been highlighted by several studies (e.g., (Hillman and Sanden 2008; Reap et al. 2008; Finnveden et al. 2009; Collinge et al. 2013)). Time can be integrated into LCI through different methodological modeling approaches (e.g., from the area of financial accounting; see Ciroth et al. (2008) for a brief review of the types of models), or can be included as part of uncertainty analysis (Huijbregts et al. 2001; Stasinopoulos et al. 2012; Collinge et al. 2013). Recently, also in line with more powerful modeling capabilities and better data availability, there is increased interest in integrating time in LCI models and create dynamic LCIs, introducing temporal parameters in processes (Tiruta-Barna et al. 2016; Beloin-Saint-Pierre et al. 2017; Shimako 2017).

3.3 Low Probability Flows of High Impact, Unknown Mechanisms

The basic LCI model is deterministic. Flows are modeled at an often-unspecified time and location, but with certainty. Some practitioners and databases add uncertainty information to flows, but this is done mainly to address the reliability and data quality of the information rather than the probability of the flow actually occurring at all. Only deterministic, fully certain flows are captured in an LCI model, while flows that occur with low probability are excluded. If these flows lead to impacts, the impact can be called risk following the classic definition in risk assessment, where risk equals probability time impact (Fig. 2.18).

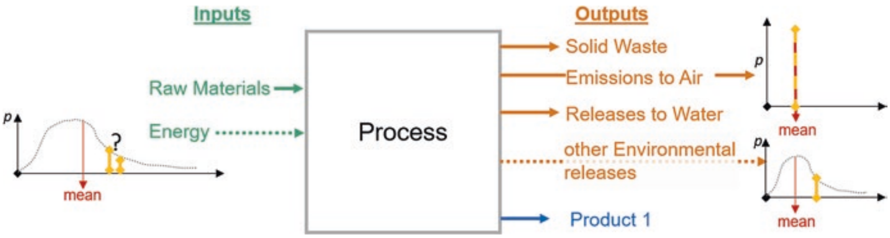

Fig. 2.18 Modeling risk in LCI: dashed arrows show uncertain flows (i.e., energy input and other environmental releases) characterized by a certain probability density function with a given mean (red arrow); the yellow lines represent the possible amount of flow occurring in the real system: these values can be far from the average for uncertain flows, while they are equal to the average for deterministic flows (e.g., for emissions to water)

In many real-life situations, flows and their subsequent impacts occur only with low probability. They are unplanned and indeterministic. Some example flows include:

– Nuclear power plants and treatment of radioactive substances with a certain, low, probability for emission of radioactive substances
– Oil leakages from oil extraction plants or during transportation via oil tankers
– Littering of plastic (e.g., determination of plastic waste path, from a source to a destination, e.g., a certain marine area)

If these flows are linked to a high impact, then this calls for an assessment of the entire risk of the process and related flow occurrence, where the risk is, as in risk assessment, obtained as a product of occurrence probability and damage, that is, environmental impact.

Slightly different cases are flows, where the behavior, their derivatives, and metabolites in the environment are simply not fully known, and accordingly, the mechanisms of these flows are currently not fully known. Examples include genetically modified organisms and nanoproducts. Nanoproducts emissions are nowadays in LCA addressed via a deterministic model, following an international workshop recommendation, summarized in Klöpffer et al. (2007):

> *"LCA gives a more holistic picture of the environmental impacts of products than does RA [Risk Assessment] alone. Furthermore, it allows the identification of the life cycle stages, the stage at which major environmental impacts may occur, and the potential risk of exposure for different people along the product-transformation chain. LCA provides very useful indications for improvement and potential impact minimization."*

Even though this earlier source also highlights the need for more information on inventory and impacts, LCA is identified as the main tool. Today, authors seem more cautious and increasingly stress that qualitative and risk-based information would be needed to complement the analysis (e.g., Curran 2015, p 49):

> *"If LCA is used exclusively to assess the environmental impact of a nanoproduct, it will adequately capture the issues related to resource management and climate change issues […]. However, shortcomings may arise because models for the underlying characterization*

of impacts to human and ecosystem health are underdeveloped […]. Thus, the incorporation of a modified risk-based health impact model accounting for chemical factors under site-specific conditions into the LCA framework would achieve a maximum understanding of the impacts of a nanoproduct to guide decisions […]".

In LCI, specific events can of course be addressed via sensitivity analysis, in which the event is described as a variation of flows (e.g., increase or decrease of a certain type of emissions). This variation can even be characterized with a certain probability. However, this approach is used to address rather few additional modeling options than full inventories that are not deterministic, and even less to model chains of consequences with probability. For these, other tools "outside" the usual LCA modeling domain exist. For instance, Bayesian networks (BN) used for failure mode effect analyses (FMEA) and risk assessment are found to be able to address questions such as the reliability of technical plants up to nuclear power plants adequately (although not as only tool to be used in practice) (Fig. 2.19).

This short discussion shows that LCI modeling is not able to fully capture the impacts of certain products. A basic LCI model has difficulties to address (i) flows that are highly uncertain in occurrence, but still important due to a potentially high impact, and (ii) flows that cause impacts that are uncertain. Both challenge the understanding that an LCA constitutes a comprehensive assessment of the potential impacts of a product over its life cycle. The second difficulty might mainly be an

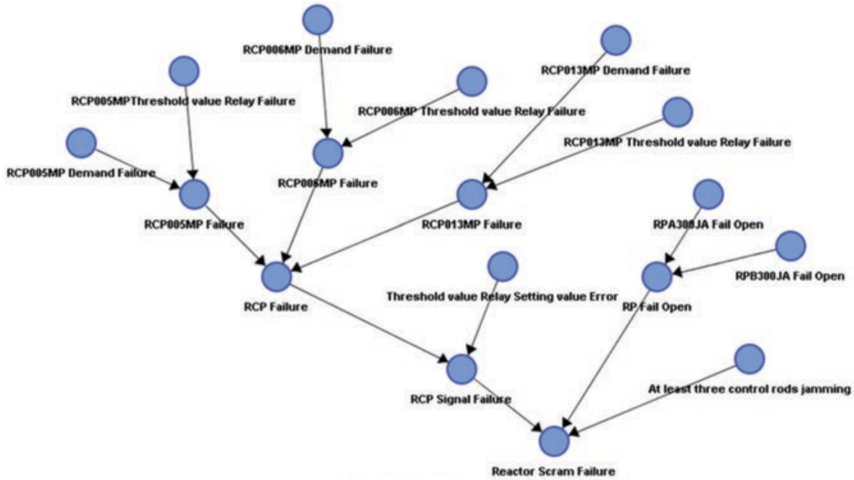

Table 1 Probability of root nodes

Root nodes	Probability	Root nodes	Probability
RCP005MP Demand Failure	6.13E-03	RCP013MP Threshold value Relay Failure	1.00E-04
RCP005MPThreshold value Relay Failure	1.00E-04	Threshold value Relay Setting value Error	1.50E-04
RCP006MP Demand Failure	6.13E-03	RPA300JA Fail Open	3.20E-04
RCP006MP Threshold value Relay Failure	1.00E-04	RPB300JA Fail Open	3.20E-04
RCP013MP Demand Failure	6.13E-03	At least three control rods jamming	1.00E-04

Fig. 2.19 A simple failure mode effect analysis for the Daya Bay nuclear power plant in Country X (Yu et al. 2003)

issue for the impact assessment phase, although the uncertain impacts of entities released to the environment may also call for a different modeling of their flows. The first difficulty is usually addressed in risk assessment, albeit not in a life cycle perspective. The inclusion of risk assessment within LCA and LCA integration with risk assessment has been debating in the last decades. Risk assessment aims at (i) identifying hazardous events that can affect some endpoint (e.g., humans, and the environment), (ii) assessing the likelihood of these events, and (iii) its potential consequences (Kaplan and Garrick 1981). First attempts to include risk in LCA were focused on chemical pollutant toxicity (human and eco) and took inspiration from knowledge in chemical risk assessment (e.g., Guinée and Heijungs 1993; Keller et al. 1998). Differences, synergies, and potential integration between these two disciplines have been extensively discussed in the literature (e.g., Olsen et al. 2001; Cowell et al. 2002; Hofstetter et al. 2002; Bare 2006). According to Harder et al. (2015), most recent studies dealing with integration between risk assessment and LCA can be classified into three main clusters: (i) site-dependent assessments, which start from environmental input-output analysis aim at assessing spatially differentiated human health risks; (ii) applications of life cycle thinking in risk assessment, which implies an enlargement of the risk assessment scope to include the entire life cycle of products; and (iii) trade-off between local and global effects, tackling the issue of burden shifting when focusing on specific contexts.

4 Life Cycle Modeling Conventions

4.1 Modeling Transport Services

Transportation is involved in most LCA studies. Modeling transportation services includes the production of vehicles, the use phase that usually involves fuel consumption and related emissions, but also construction and maintenance of transport infrastructures (e.g., roads and rails), as well as the end of life of vehicles. Transportation models involve crucial assumptions on the life span of vehicles, and average load, and average traveling or working conditions (i.e., in terms of emissions). Additionally, modeling the *use* of roads and other infrastructures by each type of vehicle requires extensive data collection, which is seldom regularly updated (Spielmann et al. 2007).

Two main LCI approaches have been developed to model transportation. The first one considers both the transported mass (e.g., a ton) and traveled distance (e.g., km). The environmental exchanges are related to the reference unit of one ton-kilometer (or kilogram-kilometer, or 1 kg over 100 km), which is defined as the transport of 1 metric ton of goods by a certain transport service over 1 kilometer. The forward and return trips can be already included in the model, and the only data to be collected are transported mass and traveled distance (usually only one-way distance). The accuracy of the model can be increased through the use of parameters

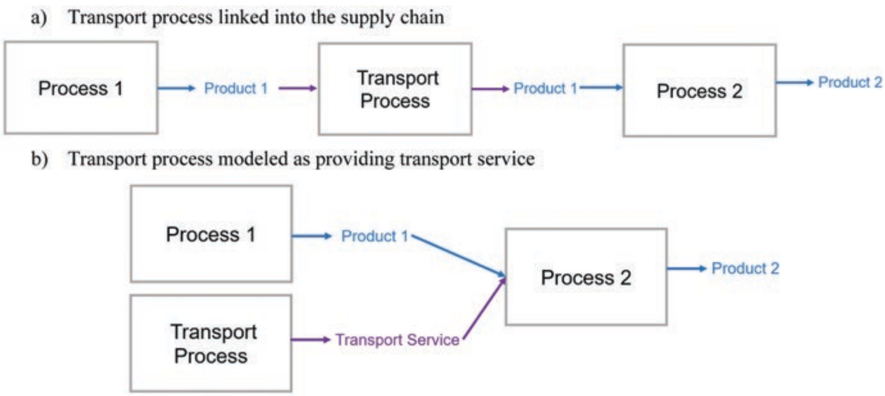

Fig. 2.20 Modeling generic transport processes as linked into the supply chain (**a**) or as a separate process providing transport service (**b**); principle example for transporting product 1 from process 1 to process 2 in a supply chain

such as level of utilization with respect to the maximum load capacity (i.e., ratio between actual load and maximum total payload), specification for forward and return trips (e.g., different loads or utilizations), and fuel characteristics (e.g., sulfur content and share of biogenic CO_2). This first model is applied to both cargo and passenger transportation.

A second modeling approach has been developed to describe passenger vehicles (i.e., cars). The functional unit is 1 vehicle-kilometer for passenger car processes. This means that the only information to be collected in the traveled distance and information about the traveled road categories, such as urban, rural, or highway, while the transported mass is not considered.

When creating the LCI model, transport can for one be modeled as service delivered to the process requesting transport, or it can be a separate process that links the process providing the product and the process "consuming" the product, so that the transport process is directly linked into the supply chain (Fig. 2.20).

Both approaches are common. Databases and software tools that request unique product names typically follow the "transport service" modeling approach, including the ecoinvent database, and SimaPro as LCA tool; the GaBi database follows the approach to link transport processes in the supply chain.

4.2 Modeling the Use Phase

Modeling the use phase in LCI is a challenging step. Usually, differently from the production process, a specific product can be used in several alternative ways. A laptop can be intensively and continuously used for working activities or just for a few times per week for leisure activities. For this reason, modeling the use phase often means developing expected average or typical consumption patterns that can highly deviate from the actual use of a single product by a single end-user. Therefore, several assumptions have to be adopted, such as lifespan of the product, number of uses, type and number of maintenance activities, as well as type and amount of energy used.

For instance, in the case of transportation, especially those requiring fuel, use phase impacts depend on assumptions regarding the lifespan of the vehicle, the average load, average fuel consumption per kilometer, and maintenance interventions (e.g., substitution of wheels and other components) (Spielmann et al. 2007). For food items, such as pasta, average cooking conditions need to be assumed. Usually, pasta is boiled for a given period of time in a given amount of water, which is heated with gas (in Italy). The time period, amount of water, and type of energy can change and the environmental impacts can therefore vary considerably (Ruini et al. 2013). Inventory processes in the use phase can be grouped into product-independent and product-dependent processes (European Commission 2018). *Product-independent processes* do not depend on the way a product is designed or distributed. They do not contribute to any differentiation between two products. For example, CO_2 emissions related to the electric grid mix, where electricity is used for boiling 1 liter of water used to prepare instant coffee is independent from the specific product design. *Product-dependent processes*, instead, are determined or influenced by the product design or use instructions and contribute to differentiation between two products. An example is the efficiency of different water boilers, that is, the consumption of more or less electricity for bringing 1 liter of water to the boiling point.

Often, modeling the use phase is related to the main function of a product, such as the electricity consumed during the utilization of electric and electronic tools (e.g., washing machine or laptop). Besides this approach, the *Delta approach* can be useful (European Commission 2018). This is applied when the use of one product influences the environmental impacts of another product, and it involves allocation. For instance, toner cartridges are not held responsible for the consumption of paper they print, but if remanufactured, the toner cartridge works less efficiently and causes more paper loss compared to an original cartridge, the additional paper loss should be allocated to the remanufactured cartridge (European Commission 2018).

The use phase can have a great contribution to the environmental impact of a whole life cycle, as for energy-using appliances (Throne-Holst et al. 2007), and the consumer behavior can significantly influence this contribution (Solli et al. 2009). This relevance was realized already in early LCA studies (e.g., Eberle and Franze 1998; Jönsson 1999). For these reasons, in current LCA practice, the use phase is typically modeled explicitly (Polizzi di Sorrentino et al. 2016). At the same time, the use phase is often not fully under the influence of the producer (e.g., how long a user takes a shower and how they set the water temperature for the shower), and it is not even easy to know since users will usually not document their behavior easily and in an accessible way. Recently, the need to go beyond average use patterns and taking into account interindividual behavioral variation while modeling different usage scenarios has been highlighted by several studies (see Polizzi di Sorrentino et al. 2016 for a review).

4.3 Modeling End of Life

Waste can occur at different points of a product system, either during the production, the distribution, or after the use phase. Modeling the waste and end of life is therefore a crucial element in LCI, but it is challenged by the dependence on waste source (which also influences the type of waste, e.g., industry or households), geographical origin, transportation (de Beaufort-Langeveld et al. 2003), waste treatment, and technology, as well as by the time lag between production and end of life (e.g., in the case of buildings). This makes the identification and description of waste treatment options more difficult.

There are two ways of modeling waste flows and treatment in LCA software (Di Noi et al. 2017, see Fig. 2.19). The first approach considers the waste treatment as a "service" for the process to eliminate the product. It is also called *opposite direction approach*, since waste treatment is added as input into the process preceding the waste treatment itself or the main process (i.e., process that delivers the reference flow or final product), and waste flow is added as a negative input, which mathematically means that it is an output. The same flow is an output in the waste treatment process.

The second approach follows the more natural direction of flows from one process to the other, meaning that the waste is an output from the production or use phase from which it is generated. In this case, a specific type of flow (waste flow) is defined and inserted as output in the waste-producing process, as well as an input in the waste treatment process.

The modeling described above refers to waste and needs to solve the problem that waste treatment processes offer a service that is "opposite" to normal production processes and thus somewhat contradict normal LCA process modeling. Normal processes produce products that are providing a value and deliver these to other processes. The product is the output of these processes. Waste treatment processes provide benefits by *accepting* waste (on the input of the process). Both the "opposite direction" and the "flow logic" approach solve this by reversing the direction of the waste flow.

Modeling recyclates, that is, substances that have been created or produced and are now used a second time, is also part of the end-of-life modeling but poses, in addition, the question of how to distribute, or allocate, the burdens over the two (or even more) life cycles. According to Baumann and Tillman (2004), some recyclate allocation methods have been framed around *fairness*, meaning which product or process is responsible for raw material extraction, waste production, and recycling. Other more *change-oriented methods* consider what would happen if the recycling system is changed. The first group includes:

(i) The *cut-off* method that assigns only direct impacts to a given product (e.g., extraction of virgin material is allocated only to the first product) and does not require data from outside the investigated life cycle.

(ii) Allocation based on the *relative loss of quality* in subsequent recycling. This method allocates environmental burdens according to the quality of the material, which is supposed to gradually decrease from recycling to recycling.

(iii) Waste is seen as a consequence of raw material extraction and thus allocated to the *first* production process that is responsible for the raw material extraction. This method promotes the *use* of recycled material.

(iv) Waste can also be allocated to the process that does not recycle, while to the processes that ensure waste recycling only the environmental burden caused by recycling is assigned. This method gives *incentives to produce recyclable products*.

The second group of methods is based on change-oriented arguments. System expansion can be the suitable approach, but given the additional data requirements and uncertainties, allocation methods that are approximations of the system expansion have been developed:

(v) *Closed-loop recycling approximation* uniformly allocates environmental burdens of raw material extraction, waste production, and recycling to all the processes involving these flows. This approximation is suitable for materials that do not lose quality when recycled and can therefore replace virgin materials.

(vi) For materials that lose quality during recycling and cannot be easily used in the same product, the closed-loop approximation is less suitable, and an alternative method is the *50–50 method* (Ekvall 1994). It assigns the burdens due to raw material extraction and waste treatment to the first and last product in the overall system (i.e., composed by the different product systems connected via waste flows) in equal proportions, and allocate the recycling process to 50% to the product upstream and 50% to the product downstream the recycling itself.

In the last years, further methods have been developed, including the Circular Footprint Formula (CFF) developed within the Product Environmental Footprint (PEF) project by the European Commission (European Commission 2018). The first version of the formula was presented in 2013, then referred to as the End-of-Life Formula. The CFF formula includes specification for material (virgin and recycled), energy (in case of energy recovery from waste), and disposal (Fig. 2.21). The general formula considers different possible material origins (i.e., virgin or recycled), waste treatment and their efficiencies, and quality of materials.

Material $$(1 - R_1)E_V + R_1 \times \left(AE_{recycled} + (1 - A)E_V \times \frac{Q_{Sin}}{Q_p}\right) + (1 - A)R_2 \times \left(E_{recyclingEoL} - E_V^{*} \times \frac{Q_{Sout}}{Q_p}\right)$$

Energy $$(1 - B)R_3 \times (E_{ER} - LHV \times X_{ER,heat} \times E_{SE,heat} - LHV \times X_{ER,elec} \times E_{SE,elec})$$

Disposal $$(1 - R_2 - R_3) \times E_D$$

Fig. 2.21 PEF Circular Footprint Formula

***A*:** allocation factor of burdens and credits between supplier and user of recycled materials; ***B*:** allocation factor of energy recovery processes: it applies both to burdens and credits; Q_{sin}, Q_{sout}, Q_p: quality of the ingoing secondary material, of the outgoing secondary material, and of the virgin material; R_1**:** proportion of material in the input to the production that has been recycled from a previous system; R_2**:** proportion of the material in the product that will be recycled (or reused) in a subsequent system; R_3**:** proportion of the material in the product that is used for energy recovery at end of life; $E_{recycled}$**:** specific emissions and resources consumed arising from the recycling process of the recycled (reused) material; $E_{recyclingEoL}$: specific emissions and resources consumed arising from the recycling process at end of life; E_v, E^*_v**:** specific emissions and resources consumed arising from the acquisition and preprocessing of virgin material, and of virgin material assumed to be substituted by recyclable materials; E_{ER}**:** specific emissions and resources consumed arising from the energy recovery process; $E_{SE,heat}$ and $E_{SE,elec}$**:** specific emissions and resources consumed that would have arisen from the specific substituted energy source; E_D**:** specific emissions and resources consumed arising from disposal of waste material at the end of life of the analyzed product, without energy recovery; $X_{ER,heat}$ and $X_{ER,elec}$**:** efficiency of the energy recovery process for both heat and electricity; **LHV:** lower heating value of the material in the product that is used for energy recovery.

The debate and research on how to tackle recycling materials are still ongoing and there is no consensus on a single approach. This topic is crucial when LCA is used, especially within the context of circular economy (Dieterle et al. 2018).

5 Conclusion

The basic LCI model is rather simple but at the same time proven to be very useful and successful in the last decades. Setting the functional unit, choosing an approach for modeling causality, setting system boundaries, and modeling locations are important aspects of the basic LCI model. The model can, however, be extended to become more realistic and to cover also more complicated production and service processes, as shown by the extensions described in this chapter. Modeling multifunctionality, time, and accidents are examples of such extensions. Whereas multifunctionality is commonly modeled through system expansion, allocation and substation in current LCA practice, the explicit consideration of time, and particularly the consideration of accidents are less common. These extensions might become more frequently applied in the future, possibly along with other extensions. If they become more frequent in the future, generic conventions for their modeling might emerge in a similar way as it already has for the modeling of certain often-occurring processes, such as transport services, the use phase, and end of life.

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Chapter 3
Development of Unit Process Datasets

Xiaojin Zhang, Hongtao Wang, and Karin Treyer

Abstract The development of unit process datasets is fundamental for any Life Cycle Assessment (LCA) study. Unit processes developed are not always of the quality desired, which impedes their usability and influences the overall credibility of the studied system. This chapter is based on the relevant LCA standards and guidelines and streamlines the detailed procedures of unit process development from a practical point of view. It aims to serve as a brief, structured, and practical guidance and suggests "basic requirements," i.e., what is necessarily required to produce a unit process dataset with reasonable data quality as well as sufficient and transparent documentation. Detailed recommendations are provided for self-checking, sensitivity analysis for improving the overall data quality, data quality evaluation, documentation, reviews, and development of tools that facilitate the development and application of unit processes. The chapter is meant to inform and aid experienced LCA practitioners from industry, policy, regulatory organizations, consultancy, and academia in unit process development.

Keywords Critical review · Data quality · Data source · Documentation · Global sensitivity analysis (GSA) · International Organisation for Standardization (ISO) · Life cycle assessment (LCA) · Life Cycle Impact Assessment (LCIA) · Life Cycle Inventory Analysis (LCI) · Missing data · Raw data · Terminology · Unit process dataset · Validation

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1 Introduction

The development of unit processes is essential in Life Cycle Assessment (LCA). All LCA modeling is based on unit processes. In general, there are four types of guidelines:

1. International ISO standards which provide the general methodology framework for LCA (International Organisation for Standardization (ISO) 2006)
2. Guidance by organizations and individuals that address the procedures for a complete LCA study (Guinée 2006; JRC EC IES 2010a; JRC EC 2018)
3. Database guidelines introducing the requirements and methodology for dataset providers (Weidema et al. 2013; Baitz et al. 2014)
4. Textbooks or handbooks with detailed instructions onto LCA (see Curran 2012; Hauschild et al. 2018)

However, these general guidelines and handbooks are not entirely applicable for the development of a unit process. Global Guidance Principles for Life Cycle Assessment Database (Shonan Guidance Principles) is the only guidance that introduces the development of unit process datasets (UNEP/SETAC 2011). This chapter is built on the basis of the general framework and requirements outlined by ISO (2006a, b) and complements the existing Shonan Guidance on unit process development. The document clarifies a few relevant terminology definitions, and diagrams are provided to illustrate the procedures for unit process development. Before getting into the procedures of unit process development, it is important to differentiate the definition of unit process dataset and aggregated process dataset.

The Shonan Guidance Principles define unit process modeling as the procedures of collecting raw data and defining mathematical relations to obtain unit process datasets (UNEP/SETAC 2011). According to this definition, when the input and output flows are based on raw data in relation to a reference product or service, these inputs and outputs form the core information required for a unit process dataset (or "unit process inventory").

Another concept that is closely linked to the definition of a unit process dataset is the aggregated process dataset. An aggregated process dataset (also known as "system process dataset" or "accumulated life cycle inventory result") is formed by combining multiple unit processes and/or other aggregated processes. Aggregated process datasets consist of accumulated flows, which can be further divided into elementary and intermediate flows. The former refers to the flows that have been drawn from or emitted to the environment without previous or subsequent human transformation. The latter refers to an output from a unit process that is input to other unit processes requiring further transformation (UNEP/SETAC 2011; ISO 2006b). Aggregated process datasets can consist of either accumulated elementary flows only, intermediate flows only, or a combination of both. Aggregated process datasets with elementary flows only can be multiplied by the characterization factors in Life Cycle Impact Assessment (LCIA) to calculate life cycle impacts (ISO

2006a), and are needed, for example, when certain details of unit process datasets are subject to data confidentiality.

This chapter is, however, focused on the development of a unit process. The general procedures in this chapter can be applied to unit processes developed for both attributional and consequential LCA modeling. The only difference between unit processes developed for attributional and consequential LCA lies in the choice of how to connect the flows.

2 General Procedures of Developing Unit Processes

The general procedure of unit process development consists of the following steps:

1. Goal and scope definition of unit processes
2. Data collection and accounting of flows
3. Matching of flows with background datasets (optional step; improves the usability of unit process; requires connection of flows with background datasets)
4. Internal check (performed by the unit process developer; e.g., based on mass balance, consistent assumptions, etc.)
5. Sensitivity analysis (optional step that improves unit processes and requires the connection of flows with background datasets and life cycle impact assessment)
6. Data quality evaluation
7. Documentation (parallel to all the other steps)
8. Critical review (external check; optional step)

The sequence and relationships between these steps are illustrated in Fig. 3.1. As shown in the figure, iterations between steps often occur, for example, between data collection, check, and data quality evaluation, or between data collection and critical review. Documentation is a step that runs parallel to all the steps, see also Sect. 2.4.

2.1 Goal and Scope Definition of Unit Processes

The development of a unit process starts with the goal and scope definition, which answers the question of what the unit process includes and represents. The quantified product(s) or service(s) provided by the unit process need to be specified, including the definition of the functional unit of the process. This is an essential step because all the other steps in the unit process development are related to the reference product. The definition of the functional unit often serves as the basis for comparison with other unit processes that fulfill the same function. The required information for defining the goal and scope for a unit processes is similar to that of an LCA study, but less extensive. A lot of information recommended by the existing guidelines for LCA studies are "good-to-have" for unit processes. In practice,

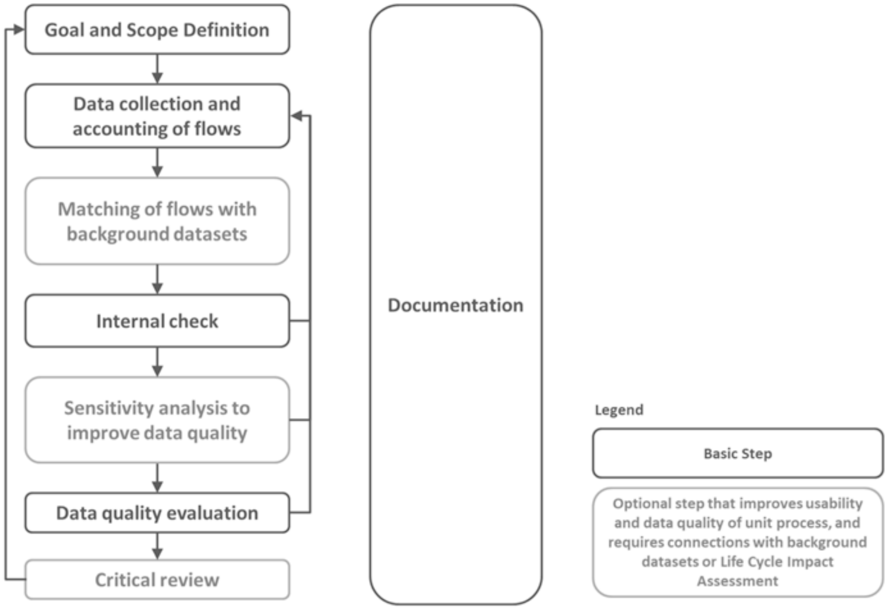

Fig. 3.1 General procedure of unit process development

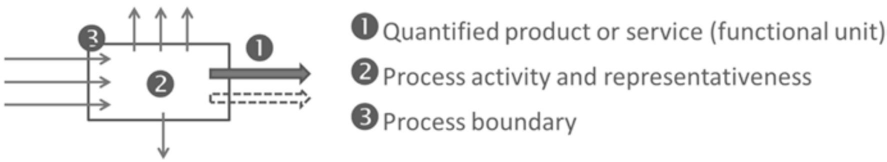

Fig. 3.2 Basic steps for goal and scope definition of a unit process

however, not all this information is always documented for every unit process. Therefore, this section suggests a key- and basic-required information to define the goal and scope of a unit process (Fig. 3.2).

First, the unit process activity as well as the product(s) or service(s) provided by the unit process activity need to be defined. The description of the product(s) or service(s) should be as specific as possible, and basic properties and classifications (e.g., size and scale, dimension, weight, shape, density) need to be provided. In multiple-product unit processes, further product properties for calculating potential allocation factors have to be identified (energy content, price, or economic value of the reference- and by-products). A quantified product or service flow is often used as the reference flow of the unit process to which all the other flows are related.

Next, the representativeness of the unit process in terms of technological, temporal, and geographical coverage needs to be defined, and it is good practice to reflect the representativeness including the following information:

- *Technological representativeness*: Technology representativeness includes information that describes the technological aspects of the unit process, such as the name of the process technology, facilities, scale, type of materials, energy supplies, waste treatment, and disposal, etc., or any other technological properties that differentiate the unit process from other aspects that produce the same product.
- *Temporal representativeness*: Usually, this can be specified by the (range of) year(s) that the unit process is intended to represent. Ideally, this is defined as the time frame for which the unit process is valid. However, the unit process developer may not always have sufficient knowledge on the temporal validity of the unit process. In this case, the (range of) reference year(s) that are valid for all raw data can be used to enable future users to better understand the dataset's approximated temporal representativeness.
- *Geographical representativeness* should include the geographical coverage for which the unit process is valid and from which the raw data for the unit process are produced (Astudillo et al. 2016). It could be as large as a world region, nation, a province/state, or a smaller area that can be specified geographically. Clear and precise definition of the geographical representativeness of a unit processes is also essential for regionalized LCA; approaches such as the Geographical Information Systems (GIS) can be applied to facilitate the definition (Mutel and Hellweg 2009; Mutel et al. 2012).

The representativeness should also define the specificity of a unit process (Weidema et al. 2004; JRC EC IES 2010b). In general, depending on how specific a unit process is, there are two types of applications: unit processes developed for producer-specific applications, and average- or generic-producer applications:

- *Producer-specific application*: The unit process developed could be used for a specific product environmental declaration, or an assessment of a product to be used for the improvement of product design, etc.
- *Average- or generic-application*: The unit process represents a group of processes that share some characteristics (technology, classification, etc.) and could, for example, be market-average or technology-representative production or service in a geographical zone.

All the above information should be clearly reflected in various fields of a unit process dataset for easy search by other users. Examples:

- Product: electricity supplied by transmission grid at 36 kV
- Activity: electricity production, high voltage
- Technological representativeness: hard coal, ultra-supercritical power plant, 1000 MW (including fuel, operating condition, size; the technology information should be ideally ranked in a sequence based on criteria such as the level of details or importance)
- Geographical representativeness: Germany
- Temporal representativeness: 2015–2020

After having defined the representativeness, the process boundary needs to be identified. Unit process boundaries specify the types of flows that are fed into or go out from the unit process. The flows included should be as complete as possible.

2.2 Data Collection and Accounting of Flows

To construct a unit process, data collection needs to be performed to understand the complete list of flows (inventory), and to account for the quantitative values of each flow. In order to obtain a complete list of flows, investigations should be made to understand what kind of flows (e.g., energy, materials, emissions, transportation, water, infrastructure, land use transformation) need to be included for the unit process, with reference to related standards and regulations, sector statistics and reports, literature, and other comparable unit processes from existing databases. Any deviations found between the flows derived from different sources should be identified and justified, both in terms of value and existence. Missing flows should be identified, e.g., by checking the balance of the unit process (Sect. 2.4). In addition, each flow should be specified with necessary details to ensure its correct and consistent correlations with other flows within the dataset (e.g., consistent conversion factors such as densities) or with flows in other datasets when the unit process is used in a larger life cycle system.

During data collection, raw data values are obtained as basis for deriving the flow values. A good and flexible unit process (i.e., a unit process that can easily be updated and customized to other projects' needs) requires careful and well-documented raw data. Raw data collected could directly be entered as the values of flows, or might need to be processed when flows are derived through mathematical relations based on the raw data as illustrated in Fig. 3.3.

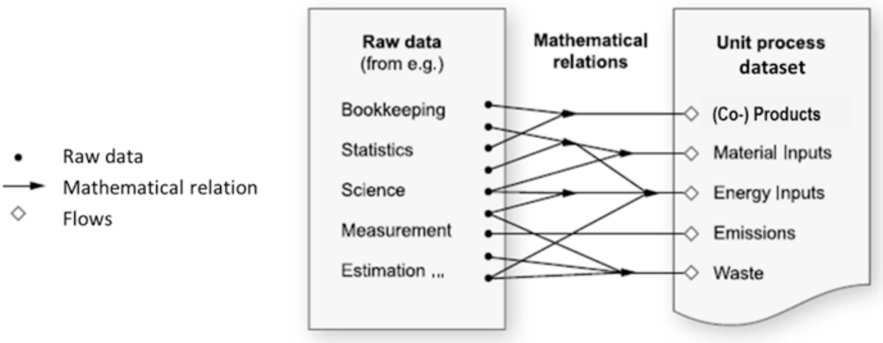

Fig. 3.3 From raw data to accounting flows via mathematical relations. (Adapted from the Shonan Guidance Principles (UNEP/SETAC 2011) with some updates in consistency with the terminology definition of this chapter)

This section discusses how to proceed from raw data collection to the accounting of flows for unit processes. First, the available raw data sources are categorized by the intended representativeness of the unit process and listed with the recommended priority from high to low. This is followed by how to deal with missing data, and then by the process of flow accounting based on raw data. In addition, there are a few types of flows which request special attention. These flows include: (1) energy carriers; (2) gaseous substances; (3) infrastructure and facilities; (4) transportation; and (5) land use and transformations.

2.2.1 Data Sources and Selection

Data sources can be different depending on how specific the intended representativeness of the unit process is. Data for a producer-specific application is usually collected from a particular manufacturer or plant, whereas the data for average or generic unit processes is often gathered from sector or governmental statistics, market reports, (public) databases, literature, etc. For the latter, the availability of data might differ depending on the country and the sector of interest. For example, major life cycle inventory data sources for various sectors in the United States are summarized in a handbook on LCA (Curran 2012), while the level of details by sectors for other countries might be different.

Some general data source examples are listed with regard to producer-specific and average or generic unit processes, prioritizing data sources from high to low in Table 3.1. The selection of data sources should closely be related to all aspects defined in the goal and scope definition of the unit process (Sect 2.1); for example, the validity of data sources used to derive the flow values should correspond to the defined technological, temporal, and geographical representativeness, and any

Table 3.1 Representativeness of unit processes with their typical data sources and priority of selecting the data source from high to low (Wang 2017)

Intended application of unit processes	Data source with choice priority from top to bottom
Producer-specific unit process	Data sources that are based on the actual supply chain or particular enterprise survey, which includes: • Measured data/bookkeeping/accounting report/Bill of Materials (BOM) with corrections based on product quality passing rate and expert inputs • Material List/BOM without corrections/Clean Production Audit Report • Environmental assessment reports, feasibility studies, or other estimates from the enterprise • Expert judgment (i.e., estimates based on the professional experience of an expert) or literature data
Average or generic unit process	• Sector statistics and report • Enterprise survey • Expert judgment or literature data

approximation or mismatch of flows should be reflected in the data quality evaluation (Sect 2.6).

2.2.2 Accounting Flows from Raw Data

When accounting the flows, multiple raw data points are preferred over single data points. When multiple raw data points are available, not only median or average values should be calculated but also the range and distribution of raw data should be included in the documentation (see uncertainty analysis).

In terms of documentation, at the level of each single flow, the value of raw data (including range and/or probability distribution) should be documented together with the source of raw data. The source of raw data should be as specific as possible, including not only the title, year, author(s) of the reference, but also more detailed information such as the page number from which the raw data is extracted. In case that raw data is not directly used as the value of flows, detailed mathematical relations should be documented to ensure the reproducibility of flow values based on the given raw data.

Mathematical Relations

The most common mathematical relations to derive flows from raw data are summarized in the following list based on both the type of mathematical relation and the raw data available:

- *Estimate based on average value* by relating the total input/output to the total amount of products produced or serviced (estimated based on median value/mode can be considered if there are enough sample points and they are more representative values given the defined goal and scope)
- *Estimate based on mass or energy balance*
- *Estimate based on modeling*, for example, on thermodynamics, chemical process engineering, system dynamics, etc.
- *Estimate based on empirical engineering formulas*, for example, formulas used in system scaling (Caduff et al. 2014)

Special Flows

A few particular types of flows are listed below. A flow associated with multiple products or services (multifunctionality) is also one of these types (see Chap. 4 of this book "Multi-functionality in Life Cycle Inventory Analysis: Approaches and Solutions").

- *Energy carriers*: Ideally, consistency should be maintained between projects and LCA practitioners as long as they refer to the same parameters (specific to the temporal and geographical scope of target). Careful evaluation of sources for such assumptions need to be done, and, whenever available, unified/agreed sources and best practices should be considered.

- *Gaseous substance*: Gas densities should be verified at the unit process level. The density applied should be specified by temperature, pressure, and other relevant parameters.
- *Infrastructure and facility*: The construction of infrastructure and facility should always be included in separate unit process datasets. However, it should be considered that infrastructure flows can be cutoff, as they do not typically contribute considerably to the results of an LCA. In such case, justification with supporting references should be provided in the documentation.
- *Transportation*: The flows of transportation should be specified by including the following information: (1) starting and ending point; (2) transportation distance; (3) weight; (4) transportation mode (e.g., lorry, passenger vehicle or shipping); (5) loading capacity; (6) model of transportation tool (e.g., vehicle type, including the energy carrier used as fuel). Starting and ending point is optional information to include, but necessary information has to be provided to ensure a clear linkage between unit process and transportation unit processes in an aggregated system. For more details on how to model the transportation service flows, see Sect. 2.4.1 "Modeling transport services."
- *Land occupation and transformation*: Land occupation and transformation receive increasing attention but is often ignored in the unit process; it is especially important for a unit process for agricultural or forestry products. For summary of land use classes see, e.g., the ecoinvent data quality guideline (Weidema et al. 2013). For land occupation, both the area and occupation duration are important to be included.

2.2.3 Flows with Missing Data

After data is collected and flows are specified and accounted, a list of flows with missing data can be identified. These flows can be categorized into two cases:

1. Flows that can be approximated
2. Flows that cannot be approximated

The first case is preferred, even if approximation might increase uncertainties. It improves the completeness of the unit process, but at the expense of reduced representativeness (Astudillo et al. 2016). Any approximation made should be reflected in the data quality evaluation.

The second case occurs when there is no alternative for reasonable assumptions to approximate the flows. However, the flows can still be "included" as part of the unit process with zero value as placeholder for future improvements. Flows with zero values should be explicitly specified in the definition of the process (Guinée 2015). It is important to enter such flows as zeros rather than simply excluding them, since this helps to differentiate these missing flows (which have not been identified) from flows that do not exist in the unit process. Additionally, it serves as a hint for potential future improvements when the data becomes available.

2.3 Matching Flows with Background Datasets (Optional)

The matching of intermediate flows with background process datasets is an optional step in the unit process development, since it involves the connection of flows with other background datasets[1], which is required to transform a unit process into an aggregated process. However, to improve the usability of a unit process in a system, it should be the responsibility of the unit process developer to specify the exact intermediate flows with a reasonable amount of details (information about the intermediate flow should be provided). This is extremely essential when unit processes are developed by individual(s), and updates to the unit process need to be made from time to time, and possibly by different individual(s).

There are occasions when a desired background dataset is not available to connect the flow. In this case, another dataset can be used to represent the dataset desired. The unit process developer – or anyone else who connects the unit process with background datasets – has to judge as to whether the approximations are appropriate. Approximated datasets are strongly recommended in case the desired dataset is not available. The use of approximated datasets should be documented and reflected in the data quality evaluation (Sect. 2.6), and should be considered in the interpretation of LCIA results. To make the unit process usable, a choice of datasets has to be provided for each flow, either by selecting approximated datasets in the background database, or by the unit process developer to construct this dataset. A usable unit process must have its flows connected with either foreground or background datasets (except if they are elementary flows).

The matching of flows with other datasets is also associated with the question as to whether the unit process is developed for consequential or attributional LCA (Ekvall 1999;Weidema 2003; Earles and Halog 2011;Habermacher 2012; Weidema et al. 2009; Zamagni et al. 2012). The use of unit processes for attributional or consequential LCA modeling determines how the flows are connected with background datasets. As defined by the Shonan Guidance Principles (UNEP/SETAC 2011), in attributional LCA, inputs and outputs are attributed to the functional unit of a product system by linking and/or partitioning the unit process of the system according to a normative rule. In consequential LCA, inputs and outputs are included in the product system, and they are expected to change, as a consequence of a change, in demand of the functional unit.

[1] Unit process datasets can be separated into foreground and background datasets. Foreground processes are directly part of the value chain of products or services in the focus of the LCA study, while the background datasets represent all up- and down-stream processes connected to the foreground datasets.

2.4 Internal Check

Various checking should be conducted by the unit process developer to improve the unit processes. This step corresponds to the "Validation" step in Shonan Guidance and can be an iterative process possibly resulting in that additional data needs to be collected, so that unit processes can be refined in terms of the values of flows and the completeness of the unit processes. The following aspects should be considered in the internal check:

- *Balance*: Balances should be checked to ensure the completeness of the unit process and to avoid, for example, unit mistakes. Balances should be followed in terms of energy, water, key chemical elements (e.g., carbon, nitrogen, and sulfur), and material flows (e.g., when no chemical reaction occurs in the unit process). The balance check requires consistent unit conversion factors, which should ideally be ensured by the tool for unit process development and can be checked automatically.
- *Consistency*: Lack of consistency can impede the usability of unit processes. Consistency should be checked regarding assumptions and mathematical relations. For example, consistent conversion factors, including densities and heating values, should be applied if they are used more than once in a unit process, or the conditions (e.g., temperature and pressure) of these assumptions should be consistent with what is defined in the unit process. Consistent mathematical relations to derive similar flows from raw data should be applied. For example, when the average value of an emission flow is calculated by relating the total emissions to the total product amount of a year, the other emission flows of the same kind should be calculated using the same approach, unless the data is not available to support the same mathematical relation applied (Lifset 2012).
- *Double counting of flows*: Double counting might occur within a unit process (e.g., double counting of particulate matter emissions of the same sizes), or between unit processes when the flows of the unit process are connected to background datasets. Any double counting should be identified in the internal check.
- *Cross-comparison with other comparable unit processes in terms of flow values*: In the definition of process boundary, references to other references are made to ensure the completeness of the inventory list. In this step, flows are compared in terms of values. Although it is not guaranteed that these comparable unit processes from existing databases and past literature are of higher confidence, any significant value differences (e.g., orders of magnitude) should be reconsidered, further checked with alternative data sources, and justified.

2.5 Sensitivity Analysis (Optional)

Sensitivity analysis is an important step to interpret and improve the robustness of unit processes but is not always performed (Mutel et al. 2013). Different from uncertainty analysis, which quantifies the uncertainty of model outputs, sensitivity analysis shows how variabilities of the model outputs (e.g., LCIA scores) can be apportioned to the different uncertainties of the model inputs (e.g., raw data or value of flows). It is recommended to perform sensitivity analysis in unit process development, as it is essential to understand the relative importance of raw data for a unit process, so as to iterate and prioritize the effort for data collection to improve data quality (Huang et al. 2012).

Mutel et al. introduced the following three types of sensitivity analysis approaches and discussed their respective drawbacks (Mutel et al. 2013):

1. One-at-a-time variation (i.e., one parameter is manually varied at a time by a certain percentage, and changes in result are computed considering this range)
2. Structure of a matrix-based LCA model (i.e., how the datasets are connected)
3. Variance of model parameters in a matrix-based LCA model

Another two-step sensitivity analysis was proposed in the end: As a first screening step to identify parameters with high sensitivities, the Method of Elementary Effects (MoEE) was applied, followed by Variance Analysis for these parameters. The advantage of this two-step approach is that it significantly reduces the number of model evaluations, and it is neither parametric nor restricted by any particular parameter distribution or mathematical structure of the LCA model.

However, to perform such a sensitivity analysis for a unit process, the flows have to be connected with the background datasets, and LCIA has to be performed. Among all these four approaches (the three listed above and the two-step approach), only the one-at-a-time variation approach can be performed using conventional LCA software, whereas the others require open-source analysis tools and coding.

In addition to the methods above, more and more applications of Global Sensitivity Analysis (GSA) appeared in recent LCA studies (Lacirignola et al. 2017; Wei et al. 2015; Cucurachi et al. 2016; Andrianandraina et al. 2015; Marini and Blanc 2014;Azadi et al. 2015; Lacirignola et al. 2014). As opposed to one-at-a-time variation, GSA considers multiple independent or correlated parameters at the same time in calculating the model outputs. This allows the ranking of input parameters and helps to identify the most influential parameters on the variability of the LCIA scores. Applying GSA in LCA can address several issues that are highly relevant to unit process development: studying the combined influence of the different input parameters, enhancing the understanding of the structure of the model, and ensuring transparency, reliability, and credibility of LCA practices (Lacirignola et al. 2017).

Several implementations of GSA in LCA are available on open-source platforms, such as in Activity Browser[2], from Kim[3] and from Groen[4] (Groen et al. 2017).

For users with access to conventional LCA software only, the one-at-a-time variation approach is recommended, and for other users with knowledge of more advanced tools and coding, the other three approaches listed above as well as GSA can be considered. In any case, sensitivity analysis is not a compulsory step of unit process development; it involves connecting the flows with background datasets and performing LCIA. However, it is a very useful step to improve the data quality and is highly recommended as good practice in unit process development.

2.6 Data Quality Evaluation

In practice, data quality evaluation is often neglected in unit process development due to time constraints. Moreover, improvement of data quality can be prioritized based on the sensitivity of flows, which cannot be estimated before the unit process is applied in an aggregated system. But data quality evaluation, either qualitative or quantitative, is important for a unit process because as soon as a unit process is used in a system, the data quality included will help to assess how uncertain the result is, which facilitates the interpretation of results and potential refinements of the LCA model.

The data quality of a unit processes can ideally be evaluated at two levels: the unit process level and the single flow level, and it can be expressed by describing: (1) how complete the unit process is (i.e., complete list of inputs and outputs), and (2) how accurate and precise the flows are. In the ecoinvent, Overview and Methodology report for version 2, the uncertainty of a unit process is categorized into four types (Frischknecht et al. 2007). Based on that, and with reference to the work of Andrae (2009) on the differentiation of data precision and accuracy, the data quality of a unit process can be categorized as shown in Table 3.2; here the first type corresponds to how complete the unit process is, and the other three types correspond to how accurate and precise the flows are. Ideally, these uncertainties should be evaluated for a unit process; however, in practice, this is often partially overlooked due to the lack of time and resources to integrate all of them. A more detailed discussion on this subject is included in Chap. 5 of this book "Data Quality in Life Cycle Inventories."

[2] https://github.com/bsteubing/lca-global-sensitivity-analysis

[3] https://github.com/aleksandra-kim/gsa_framework

[4] https://evelynegroen.github.io/Code/globalsensitivity.html

Table 3.2 General aspects and types of uncertainty in a unit process (Frischknecht et al. 2007; Andrae 2009)

General aspects	Type of uncertainty	Remark
Completeness of unit process	Neglect of flows	I.e., flows are missing due to either unavailability of data or unknown mistakes
Precision of raw data	Variability and stochastic error of raw data	E.g., due to measurement uncertainties, process variations, etc.; usually expressed by various types of distribution
Accuracy of flow	Appropriateness of the input or output flows (i.e., representativeness)	E.g., due to technical, temporal, spatial approximations
	Model uncertainty of the flow	I.e., the appropriateness of applying a mathematical relation to derive flows from raw data

2.7 *Documentation*

Documentation is important for the consistency and reproducibility of a unit process and should be performed at both unit process and flow level. It should follow the "FAIR" principles (findability, accessibility, interoperability, reusability). This does not imply that confidential information need to be disclosed to the public, but rather ensures a transparent documentation of how data have been collected and derived to form unit process datasets. Since documentation is in parallel to all other steps of unit process development (Fig. 3.1), and most information pieces required to be documented are already mentioned earlier within the other steps, only the additional information is listed below. Information should be brief and precise, quick to refer to, and identifiable by different tools (such as standardized forms, tables, bullet points, and optional lists).

The additional information at the unit process level includes:

- *Main assumptions, approximations, and limitations*: A summary should be provided
- *Review of the unit process and last modified date*

Table 3.3 shows a summary of all pieces of information that need to be documented for a unit process. This list is a general requirement for any unit process documentation. For tools (e.g., ecoeditor), more detailed fields are often required to ensure the functionality of the tool, and the ability of the unit process to be applied in software.

Table 3.3 List of information for unit process documentation, their documentation levels, and recommended types of data entry

Development procedure	Documentation fields		Level of documentation	Recommended type of data entry for documentation
Goal and scope definition	Name of unit process dataset		Unit process	Manual entry
	Quantified product(s) or service(s) (reference flow; functional unit), including properties required for calculating necessary allocation factors		Unit process	Manual entry
	Representativeness	Technological representativeness	Unit process	Manual entry
		Temporal representativeness	Unit process	Dropdown list[a]
		Geographical representativeness	Unit process	Dropdown list[a] & manual entry
	Process boundary: inclusion/exclusion of types of flows (e.g., infrastructure, transportation, etc.)		Unit process	Manual entry
Data collection and accounting of the flows	Any deviations found between the flows crossing the process boundary defined and what is included in other references or existing datasets should be identified and justified		Flow	Manual entry
	Specify the flows with a reasonable amount of details to ensure the correct and consistent connection with background datasets when the unit process is applied in a system		Flow	Manual entry
	Value, with range and distribution if applicable		Raw data	Manual entry
	Source of raw data, with a page where data comes from if applicable		Raw data	Check-box
	Mathematical relation from raw data to the input of flow		Flow	Check-box
	Flow(s) with zero value (in case background dataset is available)		Unit process	Automatic entry[b]
Matching of flows with background datasets (optional)	Approximated datasets to connect with the flow		Flow	Manual entry

(continued)

Table 3.3 (continued)

Development procedure	Documentation fields			Level of documentation	Recommended type of data entry for documentation
Internal check	Balance check			Unit process	Automatic entry
	Consistency check			Unit process	Manual entry
	Double counting of flows			Unit process	Manual entry
	Cross-comparison with other comparable unit processes, and any significant value difference is to be justified			Unit process	Manual entry
Sensitivity analysis to improve data quality (optional; iterative data collection might be needed)	Exclusion of flow(s) in case the exclusion is not sensitive to the impacts of interest			Unit process	Manual entry
Data quality evaluation	Data quality of raw data			Raw data	Table with dropdown list
	Quality of mathematical relation			Flow	Dropdown list
	Data quality of flow			Flow	Table with dropdown list
	Data quality of unit process			Unit process	Table with dropdown list
Other documentation	Main assumptions, approximations, and limitations	New unit process name		Unit process	Manual and automatic entry
		Updated unit process	Original unit process name	Unit process	Manual entry and/or automatic entry[c]
			Updates and refinements	Unit process	Manual entry and/or automatic entry[c]
	Author with contact information			Unit process	Manuel entry and/or automatic entry[d]
	Unit process last modified date			Unit process	Manuel entry and/or automatic entry

(continued)

Table 3.3 (continued)

Development procedure	Documentation fields	Level of documentation	Recommended type of data entry for documentation
Critical review	"Correctness" of the unit process	Unit process/ Flow/Raw data	Check box and manual entry
	Check performed	Unit process	Check-box and manual entry
	Data quality evaluated	Unit process/ Flow/Raw data	Check-box and manual entry
	Documentation	Unit process	Check-box and manual entry

[a]Dropdown list of time format and existing geographical zones or locations to ensure consistency
[b]Missing flows are entered as zero, thus they can be detected by the tool for unit process development and automatically filled in the unit process documentation
[c]When updates of a unit process dataset are started by copying an existing unit process dataset, the name of the original dataset and the updates can be automatically filled by the unit process development tool
[d]One-time registration and login required when working on unit process development

2.8 Critical Review

According to ISO (2006b), the critical review (Klöpffer 2012) in an LCA study is the "process intended to ensure consistency between an LCA and the principles and requirements of the international standards on life cycle assessment," which is essential to ensure the high quality of the study. The same applies to unit process development. The critical review is a step performed by external experts to ensure that all the requirements in the other steps are reasonably met.

Review of "correctness": The reviewer needs to check if all the assumptions and calculations are "correct," so that the unit process represents, to the greatest extent, what is defined in the goal and scope definition.

Review of checks performed: The reviewer needs to make sure that all the required checks listed in Sect. 2.4 are performed.

Review of data quality: The review of data quality should focus on the completeness of the flows in the unit process and on the accuracy and precision of each flow. It should also be checked (see Table 3.1) if the derivation of flows can be improved by using better data sources and the mathematical relation applied is reasonable and consistent. For the entire unit process, checks should be conducted by comparing the inventory list with other references to ensure the unit process is as complete as possible.

Review of documentation: Review of the documentation should be performed at both single flow and unit process level. Reviewers should ensure that: (1) at the flow level, each flow entered can be reproduced by the given raw data and its data source; and (2) at the unit process level, the information documented is sufficient to support users either directly or indirectly (updates or refinements). The documentation should also include any limitations and potential improvements for the unit process.

3 Tools

The selection of tools for unit process development should be considered in advance. Requirements on nomenclature and file format shall be considered before the unit process development. The tools available for unit process development include Microsoft Excel, LCA software (e.g., SimaPro, GaBit, commercial software with the user interface); openLCA (free software with user interface, open-source), Brightway2 (free and open-source LCA analytical framework, with free and open-source user interfaces such as Activity Browser, Lcopt), Ecoeditor (for ecoinvent database, free but not open-source, only for dataset creation and editing), and online platforms such as eFootprint. It is, however, worth considering future improvements of tools that can better support the unit process development and facilitate the review, such as performing automatic checks, dataset formats, with more interoperability, user-friendly documentation fields, and support for regular updates of multiple unit process datasets due to new statistics release.

4 Conclusions and Outlook

The development, documentation, and review of unit processes are fundamental for any LCA. With reference to previous standards and guidance, this chapter provides a brief summary of unit process development that aims at a basic procedure with clarifications on related terms and recommendations from a practical point of view. The importance of defining the goal and scope of a unit process is key in the development process: a thorough understanding of the target representativeness and process boundary determines the data source used to derive the flows and is fundamental for the development of a robust unit process that can be applied also by other users.

Challenges in the context of unit process development still remain, and improvements for tools that support unit process development are needed to overcome these challenges. Consistency and reproducibility should be addressed, and procedures for unit process development need to be more standardized and specific, which ensures the interoperability of unit process datasets to support LCA studies with high quality.

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Chapter 4
Multifunctionality in Life Cycle Inventory Analysis: Approaches and Solutions

Jeroen Guinée, Reinout Heijungs, and Rolf Frischknecht

Abstract This chapter gives an overview of the mainstream approaches and solutions to the problem of multifunctionality in the Life Cycle Inventory (LCI) phase. Many industrial processes are multifunctional. Their purpose generally comprises more than a single product or service. Practitioners in Life Cycle Assessment (LCA) are thus faced with the problem that the product system(s) under study provide more functions than the one investigated in the functional unit of interest. Among others, an appropriate decision must therefore consider which economic and environmental flows of the multifunctional process or system are to be allocated to which of its products and services. The discussion on multifunctionality goes back to energy analysis (a precursor of LCA), and several of today's well-known solutions for the multifunctionality problem origin from this time. There is no generally accepted solution for the multifunctionality problem, and it is even hard to imagine that there will ever be a solution. On the other hand, it is generally recognized that different solutions may considerably influence LCA results depending on the exact position of the multifunctional process in the product's flow chart. As a consequence, sensitivity analyses should be applied to test the influence of different solutions. An issue that deserves more attention is the fact that most LCA case studies so far apply one of the solutions without properly justifying where and what exactly the multifunctionality problem is and which criteria are used for determining that. In this chapter,

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these steps are therefore distinguished, explicitly aiming for more transparency in the discussion on multifunctionality approaches and solutions.

Keywords Allocation · Coproduction · Data collection · International Organization for Standardization (ISO) · LCA · LCI · Life cycle assessment · Life cycle inventory analysis · Multifunctionality · Partitioning · Recycling · Society of Environmental Toxicology and Chemistry (SETAC)

1 Introduction

Life Cycle Assessment (LCA) maps the environmental performance of a product system and is generally applied for comparing the environmental performance of alternative systems fulfilling a pre-supposed similar function. Unit processes form the building blocks of a process-based[1] LCA. Many industrial processes are multifunctional. Their purpose generally comprises more than a single product or service. As an example, zinc production from zinc ore yields cadmium as a coproduct. Another often referenced example is a refinery that produces not only gasoline, but also diesel, kerosene, heavy oils, and some more.

LCA practitioners are thus faced with the problem that the product system(s) under study provide more functions than the one investigated in the functional unit of interest. Product systems do not exist independently from each other but are all interconnected in a big economic web of processes and products. LCA experts want to isolate one product system out of this big economic web, which requires difficult decisions. Among others, an appropriate decision must therefore be made regarding which economic and environmental flows of the multifunctional process or system are to be allocated to which of its products and services.

The multifunctionality problem can also be defined in a different way. Most LCA software programs today are based on matrix algebra. The central equation of such LCA software is Eq. 4.1

$$\mathbf{g} = \mathbf{B} \cdot \mathbf{A}^{-1} \cdot \mathbf{f} \tag{4.1}$$

where

$\mathbf{f}$ is the final demand vector
$\mathbf{A}$ is the technology matrix (and $\mathbf{A}^{-1}$ its inverse)
$\mathbf{B}$ is the intervention matrix

[1] Throughout this chapter, the authors refer to the process-based LCA as conceived by the Society of Environmental Toxicology and Chemistry (SETAC) and ISO. In Input/Output-based LCA, the issue of multi-functionality and allocation is already resolved at the level of data collection.

g is the vector of environmental interventions (the inventory table) (Heijungs and Suh 2002)

In order to be able to use this equation, the **A** matrix representing the flows within the economic systems needs to be square and invertible. In the **A** matrix, columns represent processes and rows represent products (or goods, functions, and wastes). A square **A** matrix thus implies that the number of rows equals the number of columns, or in other words, there are as many products as processes. In case of a multifunctional process, a process produces more than one product or function resulting in a rectangular matrix (more rows than columns). Mathematically, the multifunctionality problem thus comes down to a rectangular **A** matrix, with more rows than columns. The solution is to decrease the number of rows or to increase the number of columns, making the matrix square again.

Most existing LCA databases today do not include multifunctional processes but have already pre-allocated them to monofunctional ones. This means that a methodological problem is mixed with data, and practitioners often cannot influence or change this methodological decision anymore. Several LCA software packages do not include options to handle multifunctionality and thus need monofunctional databases, or they do not include these options because most databases provide monofunctional process data (a clear case of a vicious circle). However, for foreground processes newly inserted by the practitioner, the multifunctionality problem may still pop-up – depending on the LCA software used – and needs to be addressed, with or without assistance by the LCA software used.

The multifunctionality problem has given rise to one of the biggest controversies in LCA theory. In doing an LCA on gasoline, the direct impacts of the refinery (from pollutants like CO_2), but also the flows to and from other processes that may lead to impacts (e.g., from oil drilling) may be argued not be attributable to gasoline only, but need to be distributed over gasoline, diesel, and all other coproducts. While this is hardly contested, the debate rather focuses on how to do this. To make it more concrete: which part of the CO_2 from a refinery is allocated to the gasoline? Different schools have provided different arguments, and none of these have been completely compelling so far. To complicate the issue, the problem does not only occur in unit processes that produce several coproducts but also in unit processes that treat more than one type of waste, as well as in processes that recycle a waste into a good. It is even not agreed if the multi-output case, the multi-input case, and the recycling case must be treated using the same principles or not. As a final note, there may even be cases of multifunctionality at the use process, where a consumer may have an outflow of reusable material, such as glass.

Within ISO (2006b), a preference order for solving the multifunctionality problem has been designed. It distinguishes several solutions, separated by clauses like "wherever possible" and "where ... cannot be established." This stepwise procedure is a clear compromise, and in practice it leaves so much freedom that LCA studies having been performed according to the ISO standard can still give conflicting results.

This chapter gives an overview of the mainstream approaches and solutions to the problem of multifunctionality in the Life Cycle Inventory (LCI) phase. The first part is devoted to a short history of approaches and solutions applied, followed by a discussion on definitions and typologies, a four steps approach to identifying and solving multifunctionality in LCA, solutions to the multifunctionality problem, and finally a brief discussion of new developments and recommendations for further research.

2 The History of Dealing with Multifunctionality

One of the first workshops on LCA was held in Leuven, Belgium (de Smet 1990) in 1990. Shortly after that landmark event, LCA as a topic was embraced by the Society of Environmental Toxicology and Chemistry (SETAC). SETAC started playing a leading and coordinating role in bringing LCA practitioners, users, and scientists together to collaborate on the continuous improvement and harmonization of the LCA framework, terminology, and methodology. A second workshop on LCA was held in Leiden, the Netherlands in 1992 (Anonymous 1992). At the Leuven and Leiden workshops, Guinée and Udo de Haes (1990) and Huppes (1992), respectively, proposed to distinguish between:

- Processes producing different economic products, i.e., production of coproducts
- Processes different waste flows, i.e., combined waste processing
- Processes transforming waste flows into an economic product (recycling)[2]

Multifunctional processes have always been addressed in LCA, also in the early LCAs, although not always explicitly. In the context of energy analysis (a precursor of LCA), Boustead and Hancock (1989; see also Bickerstaffe and Tucker 1993) adopted the “display area” in m^2 as a basis for allocation in the retail sale based on the shelf area occupied by the product sold. The latter approach was later also referred to as allocation in proportion to the function of the products by Frischknecht et al. (1991).

In their analysis of energy consumption, airborne and waterborne emissions, and accidents related to PVC (polyvinyl chloride), tin, glass, and carton beverage containers in 1974, Basler und Hoffman (1974) applied the economic value of the products as a possible basis for allocation for the electrolytic production of chlorine, one of the raw materials used in the manufacture of PVC, coproducing caustic soda and hydrogen.

In LCA studies between the 1970s and the 1990s, the most common way to deal with multifunctionality problems was to apply physical quantities such as mass and energy as basis for allocation. The units explicitly used to allocate environmental

[2] In some cases, a further distinction is made between recycling or reuse in the same system (closed-loop recycling) and in another system (open-loop recycling).

inputs and outputs associated with processes producing coproducts were: kg (most studies), moles (Anonymous 1991), and energy content (Kindler and Nikles 1980). The choice of the unit sometimes strongly influenced the allocation result. For example, the electrolytic production of chlorine – one of the raw materials used in the manufacture of PVC – coproduces caustic soda and hydrogen. Huppes (1993) calculated that 25–46% of the environmental inputs and outputs of the process of electrolysis would have to be allocated to the production of chlorine, for molar versus mass allocation basis.

Till then, multifunctionality problems mainly referred to processes producing more than one valuable product (coproduction). Combined waste handling processes have not yet been dealt with explicitly so far. Nevertheless, databases at that time (e.g., Anonymous 1984) included waste handling processes that, from origin, were multifunctional, e.g., municipal household waste incineration; how allocation was performed was not explicitly documented but most likely on an energy and mass basis, which may give disputable results. For example, imagine a household waste incinerator burning 1000 kg of kitchen waste, 10 kg of PVC packaging material, and 1 kg of discarded nickel-cadmium batteries, containing 0.5 kg cadmium. How should the resulting emissions into the air of CO_2, dioxins, and cadmium be allocated? Allocation by mass would assign the cadmium emissions nearly exclusively to kitchen refuse, while for cadmium a direct physical causation can easily be constructed (Guinée et al. 1993; Huppes 1992).

Open-loop recycling had only been specified in a limited number of studies at that time. In the SETAC workshop on LCA in 1990, two methods were proposed, as long as no better alternative is available:

1. To split the environmental inputs and outputs associated with open-loop recycling on a 50% basis between the product system studied and the other product system
2. To allocate the environmental inputs and outputs associated with the recycling process only to the product system which uses the recycled material (Huisingh 1992)

Closed-loop recycling has been discussed in three different ways. Huppes (1993) argued that multifunctionality is a property at the level of the process, while open-loop versus closed-loop is a system property. A recycling process does not “know” if it is part of an open or a closed loop. Hence, both types should be treated equally. ISO 14044 (ISO 2006b), in contrast, argues that cases of closed-loop do not present an allocation problem, because all impacts belong to the same system. Heijungs and Frischknecht (1998) analyze the case in the language of matrix algebra and conclude that closed-loop recycling typically requires allocation, but that the precise allocation details are unimportant.

So far, all solutions discussed are of the partitioning type: the impacts are distributed among the various coproducts, according to some system of “allocation factors.” But a number of other methods were already discussed at that time as well. The main line of reasoning in those other methods was to take another process as a reference that produces a product similar to the recycled product. In their *Handbook* *of Industrial Energy Analysis*, Boustead and Hancock (1979; p 292) have already proposed to credit a copper-producing system coproducing steam-based electricity "with the energy that would have been necessary to generate the electricity or manufacture the fuel with the same energy content as the co-product." At that time as well, Boustead and Hancock (1979) noted that "clearly the magnitude of this energy requirement for copper will depend on the assumed value for steam production and when making energy credits in this way, these assumed values must always be clearly stated." In a study on milk packaging, a similar approach was adopted by Mekel et al. (1990) for waste incineration coproducing electricity, and for recycling where part of the primary material "saved" was subtracted according to the quality (expressed as the economic value) of the recycled material. Heintz and Baisnée (1992) suggested generalizing this approach for "open loop" recycling, which was elaborated by Tillman et al. (1992, 1994) and Weidema (1995). Their proposals can be seen as the predecessors of the nowadays well-known "market-based substitution" approach developed by Weidema et al. (1999) for consequential LCA (see Prox and Curran 2016). In general, several terms popping up for these approaches can be noticed: substitution method, avoided burdens, system expansion.[3]

These approaches are also called "end of life recycling" and are the antipode of the "recycled content" approach, partitioning all burdens of primary resource extraction and refining to only those products requiring primary materials directly. The two families of allocation approaches "end of life recycling" and "recycled content" differ in terms of sustainability (weak and strong, respectively), risk perception (risk-seeking and averse, respectively), and burden-shifting into future (yes and no, respectively) as described in Frischknecht (2010).

In 1994, the first targeted workshop addressing allocation was held in Leiden, the Netherlands (Huppes and Schneider 1994). After this key event, the attention for the topic of multifunctionality steadily increased, which is illustrated in Fig. 4.1 by a literature count of LCA articles including "allocation" and related terms in their "Topic" description or in their "Title."[4] Despite the growing attention, the multifunctionality problem has never really been "solved" in terms of, for example, consensus on a best scientific solution (cf. Reap et al. 2008; Finnveden et al. 2009). One reason is that the discussion on solutions for multifunctionality is highly value-laden (Mill 1848; Pigou 1913, p 691; Thomas 1969, 1974; Frischknecht 1994). Game theory (van Engelenburg and Nieuwlaar 1994) and position-oriented partitioning (Frischknecht 1998, 2000) were proposed to acknowledge the value-laden nature of partitioning multifunctional processes. Attempts were made to establish a link between LCA goals on one hand and most suited allocation approaches on the other (Frischknecht 1997). Another reason is the diversity of multifunctional

[3] Whether or not all these terms refer to the same feature is a matter of debate; see Heijungs and Guinée (2007).

[4] Over the period 1995–2015, the (cleaned) Web of Science search identified 506 articles dealing with allocation in their 'Topic' and 86 articles dealing with allocation in their 'Title' on a total of about 10,000 articles on LCA in general over the same period (≈1–5%). Note that first years of new journals are generally not included in Web of Science.

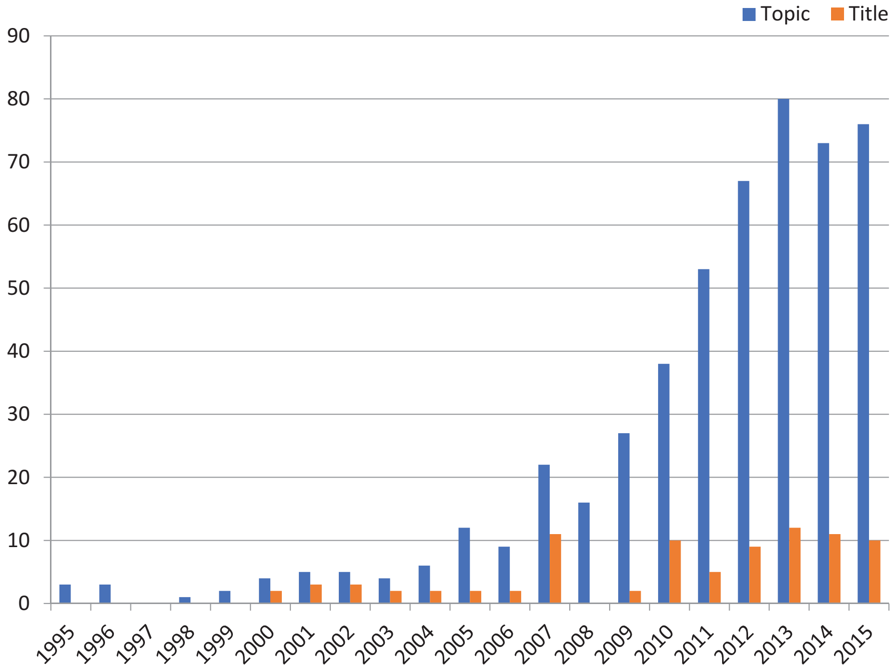


Fig. 4.1 Histogram of the number of articles (506 in total) mentioning "allocation" (or alike: multi(-)functional(ity), multi(-)product(s), coproduct(s), coproduction, multi-input, multi-output) in their "Topic" description (506 articles in total; blue bars) or in their "Title" (86 articles in total; red bars) (search result from the bibliometric analysis of the Thomson Reuters ISI Web of Science (WoS) databases on "LCA AND allocation" OR "life cycle assessment AND allocation" OR "life cycle analysis AND allocation") for the timespan = 1995–2015 (accessed on 21/12/2015). A number of mismatches were manually removed from the WoS results

processes. Basically, one can find a counter-example for every proposed solution. For instance, mass-based allocation does not work for mass-less products, such as electricity and heat, and economic value-based allocation does not work for company-internal flows for which no market price exists. A third reason is the observation by Guinée et al. (2004) that "the multi-functionality problem is an artefact of wishing to isolate one function out of many," and "as artifacts can only be cured in an artificial way, there is no "correct" way of solving the multifunctionality problem, even not in theory." Wardenaar et al. (2012) support this view by stating that "there is not an objectively correct way to solve the multifunctionality problem, but the problem can be solved in a way that serves the aim of the LCA best." They then distinguish between analysis-LCA (LCAs that are carried out for the purpose of understanding a certain system) and policy-related LCAs (supporting the regulation of the production, trade, and use of certain products), and argue that "as differences in the handling of trade-offs and uncertainties in LCAs can impede the comparability of results, it is of great importance to present clear and straight-forward applicable guidelines for such choices in a policy context." In other words, solving multifunctionality in policy-related LCA studies requires a "guideline based on robustness or consensus on best solutions for public policy applications." Despite the fact that many of the contemporary carbon footprint and other LCA-based standards now contain such guidelines, these differ between standards (even if these address the same type of footprint), and often also lack clear definitions, typologies of multifunctionality, clear systemic approach of the problems, and unambiguous solutions or solution hierarchies. ISO unfortunately also provides little guidance in this respect. Therefore, these topics are further discussed in Sects. 4 and 5. First, some definitions and typologies of multifunctional processes are briefly discussed.

3 Definitions and Typologies

Definitions of what the multifunctionality problem exactly comprises and determining criteria are mandatory for any scientific approach trying to deal with it, while often lacking in many approaches to multifunctionality today. The first definition to be introduced is on "economic flow" (Guinée 2002):

- *Economic flow:* A flow of goods, materials, services, energy or waste from one unit process to another, with either a positive (e.g., steel, transportation) or zero/negative (e.g., waste) economic value

In follow-up work, Guinée et al. (2004), building on previous work by Huppes (1992, 1993, 1994), introduced the concept of functional flow in order to define the problem of multifunctionality in an encompassing way, including coproduction, combined waste processing, recycling as well as any combination of these three typologies of multifunctional processes. They introduced several other basic definitions:

- *Functional flow:* Any of the (economic) flows of a unit process that constitute its goal (or part of its goal), viz. the product outflows (including services) of a production process and the waste inflows of a waste treatment process.
- *Non-functional flow:* Any of the flows of a unit process that are not a functional flow. These include product inflows and waste outflows, as well as elementary inflows and outflows (natural resources and pollutants).

Important is that a flow is not intrinsically a functional flow, but only with respect to a certain unit process. An outflow that is a functional flow for one unit process is a nonfunctional inflow for one or more other unit processes, and an inflow that is a functional flow for a specific unit process is a nonfunctional outflow for one or more other unit processes.

- *Multifunctional process:* A unit process yielding more than one functional flow

Bearing these definitions in mind, multifunctionality problems can be identified for each LCA study in practice by going through the following three steps (see also step 4):

1. The identification of each flow between two processes as either a product or a waste

To distinguish products from wastes, Guinée et al. (2004) suggested to adopt the economic value of flows as the determining property, again building on earlier work by Huppes (1992, 1993, 1994). A product is a flow between two processes with an economic value higher than or equal to zero, whereas a waste is a flow between two processes with an economic value smaller than zero. Note that any other criterion to distinguish between products and wastes could be applied as long as it can be consistently applied over different product systems.

2. The identification of a process' functional flow(s)

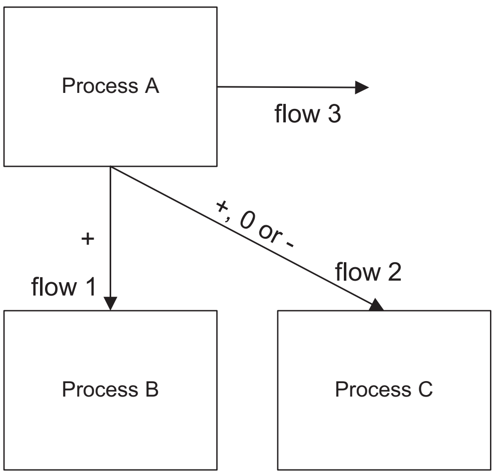
Having identified product and waste flows, the functional flow(s) of each process can now be identified, which are either products that are produced by a process or wastes that are treated by a process. Note that every process needs *at least one* functional flow.

3. The identification of multifunctional processes

Having identified the functional flows of all processes, it can now be identify which processes are multifunctional, which are those unit processes yielding more than one functional flow.

These three steps can be applied to a simple example. To determine if for process A in Fig. 4.2, there is a multifunctionality problem thus needed to know which of the three flows are functional flows. Flow 3 is an environmental or elementary flow, and therefore no functional flow, so it creates no multifunctionality problems. Assuming flow 1 has no negative value it thus comprises a functional flow for process A. If the economic value of flow 2 is higher than or equal to zero as well, it also comprises a functional flow. Process A then has a multifunctionality problem that needs to be tackled. If the economic value of flow 2, however, is smaller than zero,

Fig. 4.2 Example of a potentially multifunctional process (Guinée et al. 2004)



flow 2 would be classified as a waste. Process A then has no multifunctionality problem but flow 2 should simply be traced down to a process that will manage this flow as waste.

There can be different types of multifunctional problems. Depending on the number of functional flows and the combination of functional flows, coproduction, combined waste processing, recycling, and all sorts of combinations of these three typologies can be distinguished. Table 4.1 summarizes these typologies, while also including a monofunctional production process as well as a monofunctional waste process as references and only including one example of a combination of the three basic typologies.

Note that steps 1–3 are generally not made explicitly in most LCA studies. Most studies simply identify the problem at some point in the flowchart of their study and then apply one of the solutions. As far as these studies explain how they identified their multifunctional processes, the reasoning generally comes down to "function A belongs to system 1 and function B belongs to system 2" without providing any further criterion for this. However, as illustrated by Guinée et al. (2004), using an explicit criterion, i.e., economic value, the multifunctional problem may show up at different processes of the lifecycle, leading to different outcomes of step 1–3 and thus different case study results.

4. The solution of identified multifunctional processes; which solution(s)/method(s) are available and applicable for solving the identified multifunctionality problems?

In this fourth step, the multifunctional problem is solved by expanding the system to include an extra function, by substitution (including a negative demand of a similar function causing the multifunctional problem), or by splitting up the multifunctional process into several monofunctional processes. Options for addressing the fourth step are discussed in Sect. 4.

Table 4.1 Typologies of mono- and multifunctional processes

Typology	Example[a]	Functional flow(s)	#Functions
Monofunctional production process	g1, g2, g3 → process → g4, w1, w2	g4	1
Coproduction process	g1, g2, g3 → process → g4, g5, w2	g4; g5	2
Monofunctional waste process	w1, g1, g2 → process → w2, w3, w4	w1	1
Combined waste processing	w1, w2, g1 → process → w3, w4, w5	w1;w2	2
Recycling	w1, g1, g2 → process → g3, w2, w3	w1;g3	2
Combined waste processing and recycling	w1, w2, g1 → process → g2, g3, w3	w1; w2; g2; g3	4

[a] *g* good, *w* waste

4 Solutions to the Multifunctionality Problem

In finding solutions for the multifunctionality problem posed by the multifunctional processes identified, the mathematical formulation of the problem should be considered: a rectangular matrix, or in other words, there are more products/functions than processes or more rows than columns. In order to get a square matrix again, one can either delete a row (product or function) from or add a column (process) to the technology matrix (Heijungs and Suh 2002). This directly connects to the main approaches distinguished for solving the multifunctionality problem: system expansion or substitution, partitioning, and surplus. The authors discuss all these approaches briefly below based on the following hypothetical example.

Suppose a process incinerating 15 kg of plastic waste, producing 2 kg of slag, 140 kWh of electricity and 200 MJ of heat, as well as emitting 3 kg of CO_2, 0.2 kg of NO_x, and 150 MJ of waste heat (Fig. 4.3).

Now should be first applied step 1–3 of the identification procedure of multifunctionality problems (Table 4.2).

For applying step 1–3, it is needed to make a number of assumptions on what would happen to the flows and whether they represent an economic value or not. For a real-world example, such assumptions should of course be validated with the process owner or general public literature. Note that in specific recycling cases, the assumptions made while applying step 1–3 may make a huge difference (see Guinée et al. 2004, for example).

As discussed above, a distinction has been made in the literature between open-loop and closed-loop recycling. Open-loop recycling thereby refers to the recycling of material generated in one product system in a different product system, whereas closed-loop recycling refers to the recycling of material within one and the same product system, see ISO 14040 (ISO 2006a; Guinée 2002). Both open- and closed-loop require allocation, but for closed-loop recycling, the authors previously concluded that the precise allocation details are unimportant. Nevertheless, closed-loop recycling poses a special case that is further explored in the Appendix.

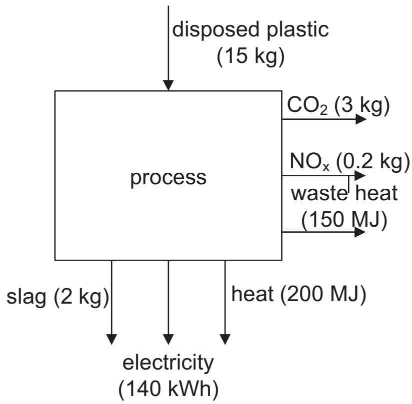


Fig. 4.3 A hypothetical process, used to illustrate the partitioning method

Table 4.2 Application of step 1–3 of the identification procedure of multifunctionality problems to the hypothetical process displayed in Fig. 4.3

1 Identification of products and wastes	Disposed plastic is a *waste*; as it is not useful anymore, it has no economic value but needs waste management
	Slag is a *waste* that needs further treatment for which the owner of the slag will need to pay the waste processor
	Electricity is a marketable *product* that can be sold to the owners of the electricity grid
	Heat appears to be a marketable *product* too, sold to heat an office building in the neighborhood
	CO_2, NO_x, and waste heat are all emitted to the environment
2 Identification of functional flow(s)	Disposed plastic, electricity, and heat are the functional flows of this process, which is thus a recycling process
3 Identification of multifunctional processes	The hypothetical process displayed in Fig. 4.3 is a multifunctional process since it has three functional flows

Having applied step 1–3, solutions for the multifunctional processes identified should be envisaged. It should be analyzed, whether there are any direct physical relations between functional flows and non-functional flows, as in the example of the household refuse incinerator burning 1000 kg of kitchen waste, 10 kg of PVC packaging material, and 1 kg of discarded nickel-cadmium batteries discussed above.

All flows for which direct physical causation cannot be established will need a different solution, of which a few are discussed in Sect. 4.1.

4.1 System Expansion and Substitution

System expansion refers to expand the system for including the additional functions. Added is an extra function to the functional unit, basically expanding the demand vector **f** (Eq. 4.1) to include more than one function ('basket of products/functions'). However, the demand vector should be qualified and quantified in such a way that it exactly matches the products/functions produced by the multifunctional process in the exact ratio as they are produced by this process. A new functional unit is then created, comprising two functions and actually answering another question (providing two functional units) than the one initially started with (focusing on one functional unit). Mathematically, the **A** matrix is still rectangular, and cannot be solved by matrix inversion, but there are then other ways to solve this (Heijungs and Suh 2002).

As discussed above, the substitution or avoided burdens method credit a process system coproducing another saleable product or function by subtracting the impacts of an alternative process system providing the same (quality of) product or function in a stand-alone way. An interesting final observation related to this topic is that the ISO standard does not mention the avoided burden approach or substitution. It does mention system expansion as a form of avoiding allocation. However, several authors (Tillman et al. 1994; Lindfors et al. 1995) have shown that system expansion and the substitution method are conceptually equivalent. That is, they do not provide the same results, but they yield results that are compatible with one another (see also Heijungs and Guinée 2007; Heijungs 2014).

4.2 Partitioning[5]

Whereas system expansion and substitution rather focus on the system of processes providing a function as a whole, partitioning takes the multifunctional process itself as cause of the problem and start of the solution. The solution is basically simple: having a process providing two products or functions, an extra column is needed, so a column is added by splitting up the multifunctional process into two (at least, when the number of functional flows of the process is two) monofunctional processes. The resulting two (or more) monofunctional processes are not existing and they may violate the laws of nature, for instance, the mass or energy balance may be incorrect. Therefore, the authors refer to these monofunctional processes as virtual processes. This splitting is here referred to as "partitioning." This partitioning can be based on several principles, which is discussed on the basis of the hypothetical example sketched above.

Several principles for solving the multifunctionality problem by partitioning can now be applied:

– Either apply a general partitioning ratio (e.g., 50%–50% in case of two functional flows)
– Apply a general principle to identify partitioning ratios (e.g., position oriented partitioning, distinguishing between competitive partitioning, and fair partitioning in coalitions (Frischknecht 1998, 2000))
– Or apply principles referring to common characteristics of the functional flows, two of which are: energy content (MJ) and proceeds (€)

The first principle is referring to partitioning based on the energy content of the functional flows, and the second is based on the economic proceeds (economic partitioning) of the functional flows. Note that mass-based partitioning in this case is not possible. This will be often the case in energy-related processes.

Now partitioning factors for each principle can be calculated according to which the nonfunctional flows of our hypothetical process are allocated to the three functional flows, eventually resulting in three virtual monofunctional processes.

[5] The multi-functionality problem is often referred to as the 'allocation problem'. Strictly speaking, allocation is not so much the problem but rather one of the solutions partitioning the non-functional inputs and outputs of a multi-functional process among its functional flows. To avoid confusion, the authors here refrain from using the term "allocation" for a specific solution and will use the term "partitioning" to refer to the specific solution.

Table 4.3 Energy content-based partitioning factors for the hypothetical recycling process

Functional flow (unit)	Quantity	Energy content (MJ/unit)	Total energy content (MJ)	Partitioning factor
Plastic waste (inflow; kg)	15	40	600	0.45
Electricity (outflow; kWh)	140	3.6	540	0.40
Heat (outflow; MJ)	200	1	200	0.15
Total	–	–	1340	1

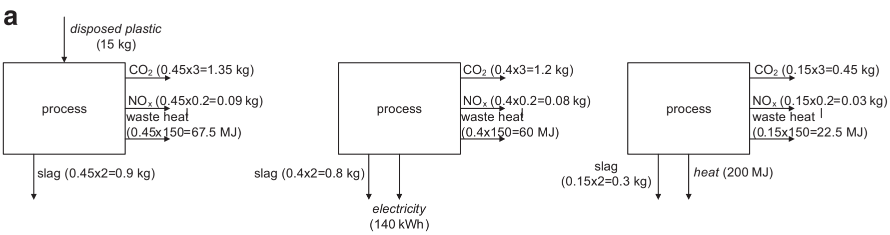


Fig. 4.4a Resulting three monofunctional process based on energy content partitioning (functional flows in italics)

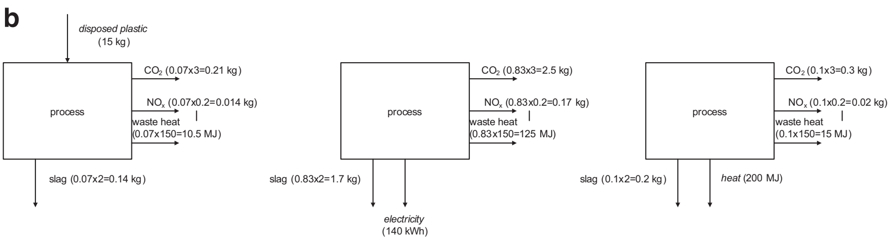


Fig. 4.4b Resulting three monofunctional process based on economic partitioning (functional flows in italics)

Table 4.3 shows the (assumed) data for energy content partitioning resulting in three monofunctional processes and data sets displayed in (Figs. 4.4a and 4.4b) (Table 4.4).

The results of this hypothetical recycling example tell that different partitioning principles can lead to substantially different partitioning results. Whether these differences matter in a specific LCA study depends, of course, on the importance of the multifunctional process in the total system studied.

For more details on economic allocation, see Guinée et al. (2004), and for other slightly different approaches of economic partitioning, see Werner and Richter (2000) and Vogtländer et al. (2001a, b). Finally, there are many other principles of partitioning possible, like mass, molar mass, area, volume, etc., but the partitioning itself works similarly for all of them as for the above examples on energy and proceeds.

Table 4.4 Economic partitioning factors for the hypothetical recycling process

Functional flow	Quantity	Price (€/unit)	Proceeds (€)	Partitioning factor
Plastic waste (inflow; kg)	15	0.2	3	0.07
Electricity (outflow; kWh)	140	0.25	35	0.83
Heat (outflow; MJ)	200	0.02	4	0.1
Total	–	–	42	1

5 Other Approaches than System Expansion/Substitution and Partitioning

Besides the main approaches discussed above (system expansion/substitution and partitioning), other approaches show up in literature. Here a few are mentioned:

Some studies (e.g., Cederberg and Stadig 2003; Guinée et al. 2009; Arvidsson et al. 2018) apply a "surplus" method, in which all impacts are allocated to the main product, and the coproducts (usually quite unimportant side products) come free of impacts. Such an approach constitutes a worst-case impact scenario for the main product with regard to multifunctionality.

Starting from the observation that a rectangular matrix needs to be inverted, tricks with the pseudo-inverse (Heijungs and Frischknecht 1998) or other least-squares approaches (Marvuglia et al. 2010) have been proposed. Their use so far is limited.

Some authors (Azapagic and Clift 1998) have used optimization procedures, for instance, linear programming for solving allocation problems. These approaches are, however, not applicable to production processes with a fixed proportion of outputs, such as chlorine-sodium production.

Because the choice of partition principle (mass, energy, economic value, etc.) can influence how a gain in symbiotic production is distributed, it has also been argued that the principle must be chosen such that all involved parties derive a fair part of the benefit (Frischknecht and Stucki 2010). So, the allocation principle becomes negotiable.

Recently, Majeau-Bettez et al. (2017) distinguished even more approaches for coproduct allocation including Alternate Activity Allocation (AAA; or "proxy-based disaggregation" assuming the technology of an alternate activity to represent the production of the coproduct to which then substitution is applied) and Lump-Sum Allocation (LSA; assuming coproducts are indistinguishable from their primary product and can be added to the primary product).

6 Discussion

The topic of multifunctionality in LCI is, after 30 years of LCA development, still an issue, and there is no sign of convergence into a widely endorsed solution. But there is a definite gain after all these years. The discussion has led to a harmonized vocabulary (see, e.g., the ISO hierarchy), a better understanding of the strong and weak points of the different solutions, a closer link to other topics in LCI (such as the overall computational structure, the distinction of goods and wastes, and the issue of system boundaries), and a better understanding of the topic from a practitioner's point of view (reflected by the fact that many good-quality LCA studies explicitly address the issue).

A further development is the recognition that the allocation problem is an artifact that derives from the desire to isolate one function from an economic web of interlinked functions. As such, only artificial solutions can be made, and there is no field validation of the results from allocation.

All proposed solutions have definite pros and cons. Tables 4.5 and 4.6 summarize the most important results of the main principles. In addition, the realm of applicability of the solutions is sometimes limited: in Sect. 4.2, an example of a case was seen where mass-based allocation did not work.

Part of the recognition of the intrinsically irresolvable nature of the problem is contrasting the use of LCA in a policy context, where standards (BSI–British Standards Institution 2008; ISO 2012; JRC-IES 2012) define the modus operandi, and the scientific context, and even add new solutions to the multifunctionality problem (JRC-IES 2012) where a case-specific discussion of the procedure needs to be carried out (Wardenaar et al. 2012). In parallel, the use of uncertainty and sensitivity analysis in scientific LCA studies becomes more and more routines. While major software packages feature at least Monte Carlo simulations, and major databases contain information on data uncertainty, the incorporation of uncertainty and sensitivity analysis in relation to the problem of multifunctionality is a relatively recent, but promising, development. In that respect, contributions by Jung et al. (2013); Mendoza Beltran et al. (2015); Hanes et al. (2015) were singled out.

Last but not least, what practitioners do in LCA case studies is often different from the theoretical considerations discussed above. Some case studies (e.g., Günkaya and Banar 2016) do not discuss the multifunctionality problem at all, which may be due to the fact that they did not face the problem or just only used data from pre-allocated LCA databases. There are also case studies (e.g., Bengtsson and Seddon 2013; Aubin et al. 2015) that only mention the allocation problem for one or two foreground processes, but not for the – much larger – background system; apparently, these authors rely on pre-allocated general-purpose databases for the background. When discussing the multifunctionality problem, the studies

Table 4.5 Results of three different solutions for the multifunctionality problem for three elements of LCA

Solution	Functional unit	System	Extra data
System expansion	Revised (for all alternatives)	Enlarged (for all alternatives)	None
Substitution	Unchanged	Enlarged (with avoided processes)	Data on avoided processes needed
Partitioning	Unchanged	Unchanged	Partitioning factors needed

Table 4.6 Additional problems of three different solutions for the multifunctionality problem

Solution	Additional problem
System expansion	You do not answer the question you started with
Substitution	Which processes are avoided?
Partitioning	What are the allocation factors?

mentioned above provide the solutions applied, but mostly without documenting any detail on how the multifunctionality problems were identified (step 1–3, Sect. 4) and only some details on how solutions were applied (e.g., calculations made and data used). Considering that the multifunctionality problem may considerably influence the results of an LCA study, lack of transparency on how this problem has been addressed will not contribute to the reproducibility and credibility of such LCA studies.

7 Conclusions and Recommendations

As argued above, the multifunctionality problem is an artifact of wishing to isolate "one function out of many," and "as artifacts can only be cured in an artificial way, there is no 'correct' way of solving the multi-functionality problem, even not in theory" (Guinée et al. 2004). There is indeed no generally accepted scientific solution for the multifunctionality problem, and it is even hard to imagine that there will ever be a solution. What comes closest is the general recognition that for consequential LCA system expansion and substitution are most appropriate solutions whereas for attributional LCA partitioning and other approaches are more suited solutions (European Commission 2010), but even this is not generally recognized and violated by many case studies (Thomassen et al. 2008). There are, however, "agreed" solutions for specific applications; as mentioned above, this applies to several footprint standards.

At the same time, it is generally recognized that different solutions may considerably influence LCA results depending on the exact position of the multifunctional process in the product's flow chart. Standards "solve" this issue by prescribing one specific solution; LCA studies for other nonstandardized applications can only sensibly deal with this issue by applying sensitivity analyses whenever more solutions are valid or can be defended.

Most case studies so far apply one of the solutions (step 4, Sect. 4) without first properly justifying where and what exactly the multifunctionality problem is and which criteria are used for determining that (step 1–3). Guinée et al. (2004) showed that this is particularly the case for recycling situations and that it may also considerably influence the results of an LCA study. It is therefore suggested to distinguish these steps explicitly in order to increase the transparency in the discussion on multifunctionality approaches and solutions.

A complicating problem when trying to increase transparency is that many databases have "solved" multifunctionality as part of their data. Currently, it would need huge efforts to implement new solutions in standards, see the EU Product Environment Footprint (PEF; European Commission 2013), and in LCA databases, such as ecoinvent, if this would be required. For instance, the equations for dealing with recycling as imposed by the EU PEF (JRC-IES 2012) would require a substantial adjustment in LCA databases and would create interlinkage between primary and secondary material supply chains. Clearly, separating multifunctionality solutions (methods) from databases (data) would solve a lot of these problems. Further, it would solve potential inconsistencies between multifunctionality decisions for background and foreground processes and enable sensitivity analysis by switching to other allocation methods or partitioning principles. Versions 1 and 2 of the ecoinvent database included separate unallocated databases, but these were hardly used because most LCA software could not handle them and obviously users were not demanding for it. The continuous rise of new solutions for allocation even as part of standards such as the EU PEF represents a strong case for separating method choices from data that, as a result, will also increase the flexible use of databases. Further research is recommended as to whether it is possible and desirable to separate method choices from databases, and what consequences this would have for LCA software programs. One thing is for sure: opening up this issue would increase transparency on how multifunctionality problems are addressed in LCA studies (and databases) and also increase the credibility of LCA, even if by opening the eyes of people that are currently ignorant of the influence of this problem in LCA and its databases. It is desirable to go to a future in which no more case studies would write that no allocation problems showed up without having a clear justification for such a statement.

Appendix: The Special Case of Closed-Loop Recycling

Suppose a system of two processes, process 1 and process 2 (Fig. 4.5), of which process 2 produced a product (i.e., recycled material) from a waste inflow. For the sake of simplicity, all other flows of both processes are left out, but in practice there will of course be other flows.

Process 1 has one product as inflow as well as one product and one waste as outflows; it thus has one functional flow and is thus a monofunctional process, no allocation needed. Process 2 has one waste as inflow and one product as outflow; it thus has two functional flows, is a multi-functional process, i.e., a (closed-loop) recycling process, and thus requires allocation (note that waste is a functional flow for process 2 but a non-functional flow for process 1). As a result of allocation, process 2 is split up in two virtual processes: process 2a, which represents a monofunctional waste process, and process 2b, which represents a monofunctional production process of recycled material (Fig. 4.6).

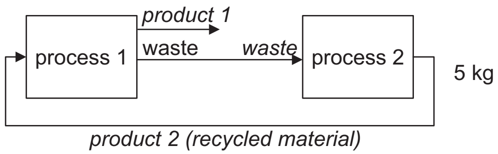


Fig. 4.5 Hypothetical system of two processes constituting an example of closed-loop recycling (functional flows in italics)

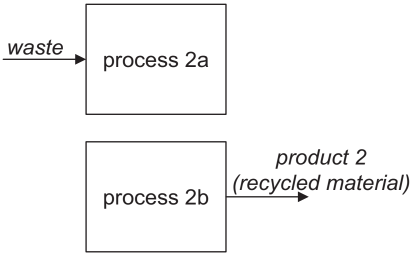


Fig. 4.6 Result of splitting up process 2 is two virtual processes: process 2a, representing a monofunctional waste process, and process 2b, representing a monofunctional production process of recycled material (functional flows in italics)

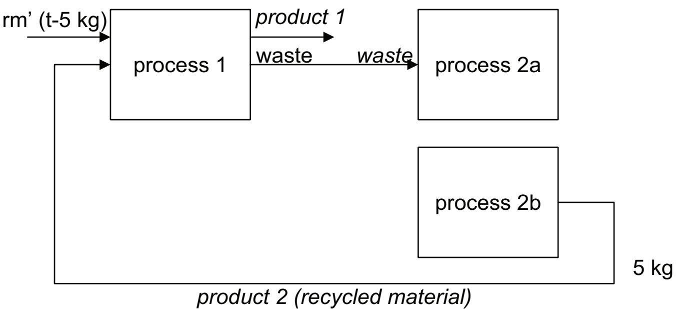


Fig. 4.7 Total demand (t) of recycled material (rm)by process 1 is >5:extra inflow needed in process 1 providing t-5 kg of similar material as rm (rm') (functional flows italics)

As a result of this allocation, now the problem is faced that in the modeling of closed-loop recycling the demand of product 2 from process 2a does not necessarily have to match the demand of product 2 by process 1, while in the real-world process demand and supply of recycled material in a closed-loop situation should exactly match. This is an important constraint of closed-loop recycling that should be kept in mind. If more recycled material is needed by process 1 than can be supplied by process 2, i.e., 5 kg, another flow should be added to process 1 providing the same material (either primary material or the same quality of recycled material but provided by another recycling process); see Fig. 4.7.

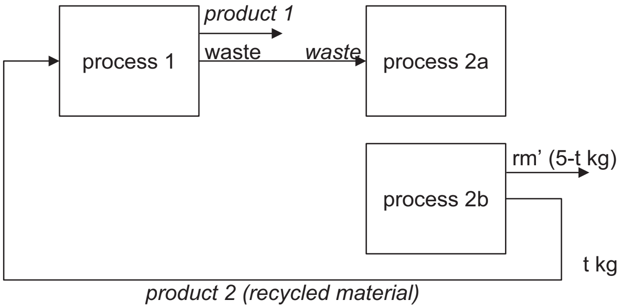


Fig. 4.8 Total demand (t) of recycled material (rm) by process 1 is<5: extra outflow needed in process 2b providing 5-t kg of rm for other product system (i.e., partial open-loop recycling) (functional flows in italics)

If less recycled material is needed by process 1 than can be supplied by process 2, i.e., less than 5 kg, another flow should be added to process 2, representing partial open-loop recycling to another product system of the remainder material; see Fig. 4.8.

The lesson learned is that for closed-loop recycling, allocation does not matter in theory *as long as* supply of the recycled material by process 2 and demand of the same material by process 1 exactly balance.

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Chapter 5
Data Quality in Life Cycle Inventories

Andreas Ciroth

Abstract This chapter explores data quality in life cycle inventory (LCI) datasets and calculation results, introduces the history, explains the relevance of data quality for life cycle assessment (LCA), and the difficulty to deal with the application-dependency of data quality. Recent data quality systems, introduced by the United States Environmental Protection Agency (US EPA) and in the course of the European "Product Environmental Footprint" (PEF) project, are elaborated in more detail. The application-dependency of data quality has led to a more refined view on data quality in a recent United Nations GLAD (Global Life Cycle Access to Data) project. GLAD distinguishes between data quality when a dataset is created and when it is used. In addition, data quality is broadened by including modeling details that are typically set differently in different application contexts. Outcomes of the GLAD project are therefore introduced in this chapter as well and it is expected that these might lead to a more comprehensive, better management of data quality for differing application contexts, as well as for creating inventory datasets.

Keywords Application-dependency · Fitness for purpose · Data quality indicators · GLAD (Global Life Cycle Access to Data) · International Reference Life Cycle Data System (ILCD) · ISO 14025 · Life cycle assessment (LCA) · Life cycle impact assessment (LCIA) · Life cycle inventory (LCI) analysis · Product category rules (PCR) · Product environmental footprint (PEF) · Product environmental footprint category rules (PEFCR) · United Nations Environment Programme (UNEP) · United States environmental protection agency (US EPA)

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1 Data Quality: An Issue in Life Cycle Inventories

Since its very beginning, life cycle assessment (LCA) method development was concerned in providing good decision support, and addressed concerns related to the quality of data used in LCAs. For example, the "Technical Framework for Life Cycle Assessment" recommends the development of data quality standards for LCA database development (Fava et al. 1991, p. 151). An international working group on LCA data quality stated as motivation that "some of these [early] LCAs have been criticized because of concerns about the quality of data used in the study" (Fava et al. 1994, p xvii).

Today, the ISO standards 14,040 and 14,044 provide an accepted definition of data quality in the LCA context, which follows the definition of quality, common in other disciplines, and broadly used standards, e.g., ISO 9000: 2015.[1] Per this definition, LCA data quality is not a static property of data, as is, for example, the creation date, but instead depends on stated (specified) requirements that are typically application-dependent. This definition and concept apply both to LCA studies and datasets in the LCA context, thus also to life cycle inventory (LCI) analysis.

Nowadays, different concepts and approaches for data quality exist in LCA and LCI. Some of these, but not all, explicitly address requirements for the application of data. Broadly speaking, these concepts differ in the following aspects:

1. The accepted and foreseen purpose for using datasets
2. The way to assess data quality, which is sometimes, in line with the ISO definition of data quality (fitness for purpose)
3. The way to store and document data quality
4. Elements needed for assessing data quality

This chapter explores aspects of data quality for LCI. It defines data quality and its role in LCA and provides an overview of current indicators and "metrics" for managing data quality in LCA, for datasets, databases, and studies and presents their application.

2 Definition of Data Quality and Fitness for Purpose

In the context of LCA and LCI, data quality is defined in ISO 14040 as *"characteristics of data that relate to their ability to satisfy stated requirements"* (ISO 2006a, sec. 3.19). Thus, the quality of a given LCI model, of datasets, or of a database, fully depends, according to ISO, on the "stated requirements." Changing requirements will change the quality of given data. Further, the ISO definition implies that sufficient information is provided to understand whether the "stated requirements"

[1] Quality management systems – Fundamentals and vocabulary (ISO 9000: 2015); German and English version EN ISO 9000:201

are met. This in turn means that the requirements need to be specified (stated), and information needs to be provided to understand to which extent these requirements are met.

Since "quality" has, for laypersons, and in contrast to the technical definition used in the ISO standards, always a positive connotation, the steering committee of the UNEP (United Nations Environment Programme) working group "Global Network of Interoperable LCA Databases" recommended the term "fitness for purpose" instead of using "data quality."[2] The definition "fitness for purpose" follows the definition of data quality (see Sect. 1), which means that fitness for purpose and data quality are synonyms.

3 Addressing Data Quality in Life Cycle Assessment

3.1 Relevance of Data Quality in LCA

As mentioned in Sect. 1, data quality is one of the key concerns for LCA, since its beginning around 1970–1990. Even the early LCA reports recognized that data quality is a cross-cutting issue, relevant for each single modeled process dataset, but also for modeling process connections as well as the full life cycle inventory and thus for a complete LCA study (Bretz 1998). LCA databases which emerged after the initial method papers also contributed to the development and broader use of data quality metrics. Many users request a "quality-assured" database, and databases announce, as key assets, to provide "high quality"[3] or "best quality" datasets.[4] Data quality was also an issue for impact assessment in LCA (Fava et al. 1994).

According to ISO 14040/14044, a critical review needs to address data quality in LCA case studies (Klöpffer 2012). The ISO standards 14,040 and 14,044 request "initial data quality requirements" to be specified in the goal and scope phase of an LCA study (Curran 2017), and data quality in the interpretation phase (Ciroth 2017). The critical review, according to ISO 14040, requires for comparable case studies to ensure that "data used are appropriate and reasonable in relation to the goal of the study" (ISO 2006a, sec. 6.1). Following the definition of data quality, this basically means to investigate whether the data quality of the study is sufficient.

[2] Global Network of Interoperable LCA Databases – Global LCA Data Access, Brasília meetings. 13–16 March 2016, Summary of decisions by Steering Committee from Brasília meeting, UNEP 2016

[3] "Our high-quality LCI datasets are based on industrial data […]," https://www.ecoinvent.org/database/buy-a-licence/why-ecoinvent/why-ecoinvent.html

[4] "European Commission: GaBi energy data has the best quality," http://www.gabi-software.com/news/news-detail/article/european-commission-gabi-energy-data-has-the-best-quality/

3.2 The Janus Property of Data Quality

So, how is data quality determined in LCA? Consider a process dataset. When creating the dataset, the modeler has typically in mind a given product and production "route" in a given location and at a given time. The modeler also has further aspects in mind such as supported LCIA methods, modeling procedures for waste and biogenic carbon, completeness requirements, and so on. For example, the targeted product can be sesame, produced in India, with conventional agriculture in 2018.

More generally, a goal and scope is specified for the dataset to-be created, just as specification of goal and scope is the first phase when performing an LCA study (Curran 2017; Sonnemann and Vigon 2011). For a dataset, these goals are the requirements mentioned in the definition of data quality. If the final dataset fully meets these goals, it is of perfect data quality.

Many databases and projects that develop and maintain larger sets of datasets define methodological guidance principles (Weidema et al. 2013) or data quality principles (Masoni et al. 2014; Kupfer et al. 2017) to harmonize the development of the datasets and to make the created datasets more consistent. By doing so, they implicitly specify the goal and scope for the datasets so, for example, related to flow nomenclatures and other overarching modeling principles. These goal and scope settings still allow different products and processes, as long as the goal for the dataset is – apart from a given nomenclature and other overarching aspects of data quality – the modeling of one specific product. As a result, databases are then able to declare and document the achieved data quality for each single dataset. This is one side of the data quality, namely, the data quality when creating datasets.

The other side of data quality becomes important when datasets are used in LCA studies, as part of the background system, or as basis for a modified dataset that then reflects a process in the foreground system.[5] For these cases, requirements will commonly be different from the requirements specified for the database, valid when the datasets were created. Now, for a specific project case, the product might, for example, not be exactly the same as the one targeted in the database (e.g., not sesame in conventional production in India in 2018, but organic sesame production in 2017 in the United States), or the year, or region, might be slightly different. Therefore, for applying a data-based set in a study, the data quality might be different from the quality documented by the database, for the same dataset. This has been called a "Janus" property of data quality, meaning that data quality for a dataset has two sides; one when the dataset is created, and one when the dataset is used (Fig. 5.1). Both can be different (Ciroth and Vigon 2016).

In practice, for an LCA study which uses many different datasets, from databases and also from other sources, the "effective" data quality for datasets cannot be taken

[5] See Chap. 2 in this book "Principles of Life Cycle Inventory Modeling: The Basic Model, Extensions and Conventions" by Andreas Ciroth, Francesca Recanati, and Rickard Arvidsson for more details about foreground and background systems in LCA.

Fig. 5.1 Janus, Roman coin, 220 BC (Ciroth and Vigon 2016)

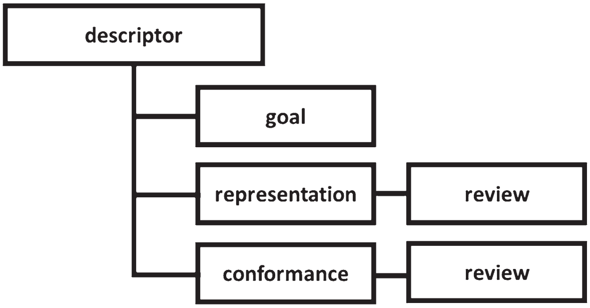

Fig. 5.2 Structure of a data quality descriptor (Ciroth et al. 2017)

directly from the database; rather, it needs to be assessed considering the use of the dataset in the study context.

3.3 Components of Data Quality Descriptors

The definition provided above already indicates that data quality consists of several elements: a goal/specification of requirements, and an ability to cope with these stated requirements, or rather an assessment of this ability, which in turn is based on what is contained or "represented" in a given dataset. This representation may of course be different from the targeted, ideal situation foreseen in the stated requirements.

Since there are several different requirements, there are also different aspects or topics addressed in data quality; each of them can be handled and evaluated with a so-called data quality descriptor. For all of these data quality descriptors, three elements are significant (Ciroth et al. 2017; Fig. 5.2):

- A goal and scope
- A "value" and representation
- A conformance, assessed as a deviation from goal and scope

Fig. 5.3 Data quality descriptor reference “time,” in the creation and application of a dataset

The conformance is the “fitness for purpose” of the dataset. While the goal is specified by the user or dataset creator, the representation (what is really contained in the dataset, e.g., which product, which region does it represent), and the conformance can be checked and reviewed. It can also be scrutinized whether the dataset is indeed of, for example, very good data quality since the representation matches well with the goal, for a given descriptor (Fig. 5.2).

Considering the Janus property of data quality, Fig. 5.3 shows the structure of a descriptor with a dataset creation and a dataset application side, and the descriptor “time.” The dataset of 2017, which was the goal for the dataset creation, yields a very good data quality, while in the application the same representation gives only a good data quality, since the goal for the application is a dataset valid for 2018.

As a consequence, conformance and data quality assessed when creating a dataset becomes less important when applying a dataset, at least for the descriptor reference “time.”

3.4 Data Quality Topics in LCI and Generic Indicators

Which aspects are overall covered by data quality? ISO 14044 lists topics that “should” be addressed in goal and scope, and “should” be addressed in comparative assertions (i.e., comparative LCA case studies) intended to be disclosed to the public (ISO 2006b, sec. 4.2.3.6; Klöpffer 2012). In ISO 14044, the topics of the requirements for data quality are:

(a) Time-related coverage: age of data and the minimum length of time over which data should be collected
(b) Geographical coverage: geographical area from which data for unit processes should be collected to satisfy the goal of the study
(c) Technology coverage: specific technology or technology mix
(d) Precision: measure of the variability of the data values for each data expressed (e.g., variance)
(e) Completeness: percentage of flow that is measured or estimated

(f) Representativeness: qualitative assessment of the degree to which the data set reflects the true population of interest (i.e., geographical coverage, time period, and technology coverage)
(g) Consistency: qualitative assessment of whether the study methodology is applied uniformly to the various components of the analysis
(h) Reproducibility: qualitative assessment of the extent to which information about the methodology and data values would allow an independent practitioner to reproduce the results reported in the study
(i) Sources of the data
(j) Uncertainty of the information (e.g., data, models, and assumptions)

This list is a good starting point for understanding data quality indicators. A disadvantage is that this topic is not really structured, and some of the indicators seem to overlap: uncertainty is listed interestingly in addition to precision.[6]

As an attempt to structure this seemingly fuzzy area, several topics can be distinguished:

– Representation and conformance aspects (time, geography, technology)
– Modeling-related aspects (selected nomenclature, modeling waste, biogenic carbon, multi-functionality)
– Measurement related aspects (completeness, reliability of the source, uncertainty of data)
– Procedural aspects (review procedure, copyright)

3.5 Data Quality Use Cases – Frameworks

Over time, several frameworks have become established where data quality is addressed. The frameworks differ in their understanding and definition of data quality, in the objects they assess, the selected data quality indicators, the assessment procedure, the aggregation of data quality, and in how data quality is applied, especially whether a minimum threshold for data quality is foreseen. Some of the most notable frameworks are presented in the following sections.

3.5.1 Data Quality in the Environmental Footprint

The Environmental Footprint (EF) is an initiative of the European Commission. It started around 2010 with the idea "*to ensure that consumers receive reliable information on the environmental performance of products*" (European Commission 2011), by establishing common modeling rules, several thousand consistent and

[6] It is not entirely clear, but "uncertainty," as mentioned in ISO, may include both random uncertainty and variability; it seems intentionally vague and broad ("… the information (e.g., data…)")

Table 5.1 Data quality structure in EF

<table>
<tr><td colspan="2">Data quality criteria</td><td>Technological representativeness
Geographical representativeness
Time-related representativeness
Completeness
Parameter uncertainty
Methodological appropriateness and consistency</td></tr>
<tr><td rowspan="3">Additional aspects</td><td>Documentation</td><td>Compliant with ILCD format</td></tr>
<tr><td>Nomenclature</td><td>Compliant with ILCD nomenclature (e.g., use of ILCD reference elementary flows for IT compatible inventories)</td></tr>
<tr><td>Review</td><td>Review by “qualified reviewer”
Separate review report</td></tr>
</table>

Recchioni et al. (2013)

rule-compliant background datasets, and almost 80 detailed test cases on a variety of products, from pasta to uninterrupted power supplies.

To achieve reliable information, several measures are taken in the EF, which have been revised and modified over time, often without public documentation (Table 5.1).

Despite a huge literature and frequent revisions, it is probably reasonable to structure the EF measures in a way that all belong to one of the following three aspects:

- *Rules*: Modeling of the life cycle follows rules which are developed per product categories, very similar to the approach adopted in environmental product declarations, namely with generic category rules and with rules specific for each addressed product group
- *Data quality assessment*: For datasets, a data quality assessment is performed, and six data quality indicators are evaluated and aggregated
- A *review* is performed for entire models, the background datasets, and also for datasets contained in the models

These three different aspects are summarized below.

The Category Rules

The product category rules in the EF (Product Environmental Footprint Category Rules – PEFCR) are meant to “*provide specific guidance for calculating and reporting products’ life cycle environmental impacts*” (European Commission 2016, p. 10). For each product group, category rules are to be developed in a multistep procedure (Fig. 5.4). This procedure, i.e., the development of product category rules in the EF, is based on the requirements in ISO 14025.[7] Even if the PEF procedure may leave the criterion “most relevant” undefined, which is crucial for the

[7] Environmental labels and declarations – Type III environmental declarations – Principles and procedures

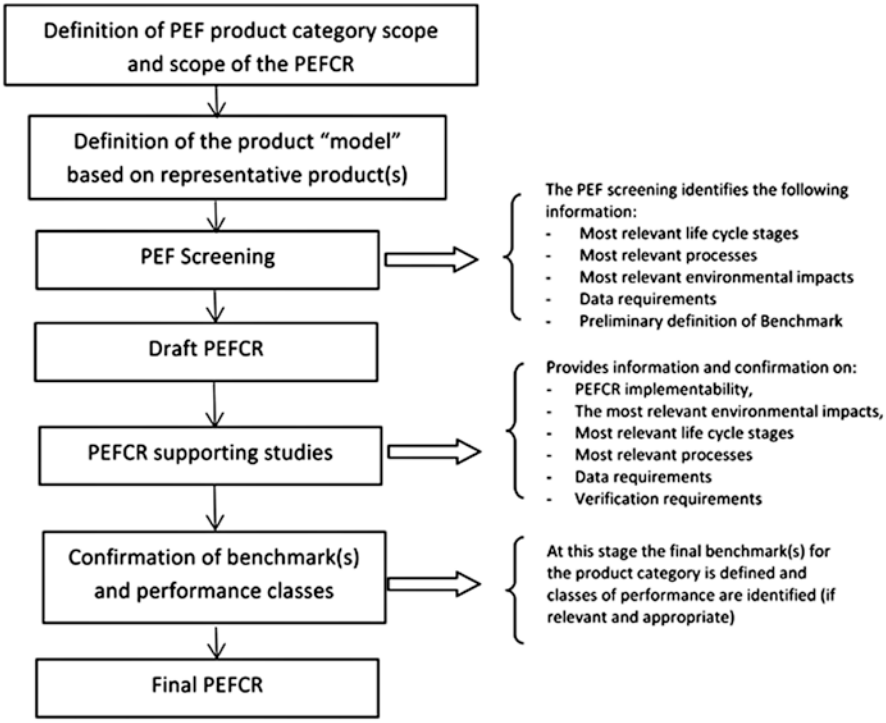

Fig. 5.4 Development of PEF category rules, PEFCR (European Commission 2016)

procedure and requires an assessment, it is overall straightforward. The PEF procedure is to be able to identify benchmarks for product comparison, to specify modeling rules for the life cycle model,[8] and it is based on broader "supporting studies".

These modeling rules include, very similar to "normal" Product Category Rules (PCR) following ISO 14025, specifications for the functional unit, system boundary settings, selection of the LCIA indicators, further assumptions, data quality requirements for the inventory, for foreground data collection, for the use of background databases, for the treatment of data gaps, for using stage modeling, for modeling transports, end of life, and for dealing with multifunctional products and processes.

In the further evolvement of the EF, a generic PEFCR has been developed (European Commission 2018a), which was complemented by specific PEFCRs for each of the targeted product groups (e.g., European Commission 2018b). For the category rules, the definition of the product group which is to be assessed by these

[8] In the EF hotspot analysis, "most relevant" is defined: Processes ordered by their contribution are most relevant up to the 80% percentile, i.e., if the sum of the impacts is equal or higher than 80% of the total impact (i.e., sum of all the impacts after normalization and weighting), see http://ec.europa.eu/environment/eussd/smgp/pdf/PEFCR_guidance_v6.3.pdf (page 50)

common rules is of course crucial, and the PEFCRs give considerable space to this topic.[9] In addition to specific modeling rules, the PEFCRs also specify general requirements regarding the documentation and the nomenclature of processes and flows, which have to be in line with requirements set forward in the International Life Cycle Data (ILCD) format developed on behalf of the EC and in the ILCD network to store and distribute LCA datasets (see Chap. 6 in this book "Life Cycle Inventory Data and Databases" by Andreas Ciroth and Salwa Burhan). Going back to the definition of data quality, the category rules define the goal (the stated requirements), and thereby implicitly harmonize and align the requirements for LCA.

The Data Quality Assessment Formula

In the EF, a data quality assessment formula is to be used for process datasets, both in the aggregated and disaggregated state. The formula consists of four elements (European Commission 2018a):

$$DQR = \frac{\acute{Te}_R + \acute{G}_R + \acute{Ti}_R + \acute{P}}{4}$$

where

DQR means data quality requirement
Te_R refers to technical representativeness
G_R refers to geographical representativeness
Ti_R is the time representativeness
P is the precision, each averaged over the dataset

These indicators represent the "classic" data quality indicators, also mentioned in ISO 14044 (see Sect. 3.4). They are determined according to Table 5.2 (if the dataset is company-specific, the assignment of scores slightly differ from the general rules reported here, e.g., scores 4 and 5 are not applicable).

It is emphasized that individual PEFCRs may be stricter and can then overrule the general assessment table (European Commission 2018a).

As the table shows, the assessment is always qualitative, also precision is measured in a qualitative way and provides best results if data is measured/calculated and externally verified. An interesting aspect is that the indicators are to be assessed on the "most relevant" aspects, which are processes for a product system, and elementary flows for process datasets. As the formula shows, the indicators are meant to be averaged, and they need to be averaged over the "most relevant" elementary flows or process datasets, respectively, which in turn are determined by the contribution to impact assessment results (European Commission 2018a, p. 177):

[9] In the development of various PEFCRs, some could not be finished since an agreement on the definition of the product category could not be reached; for example, for coffee, it is a question about the size of the cup (Americano vs. espresso) and whether milk should be included or not.

Table 5.2 PEF data quality assessment for secondary datasets

Score	P_{EF} and P_{AD}	$Ti_{R\text{-}EF}$ and $Ti_{R\text{-}AD}$	$Ti_{R\text{-}SD}$	$Te_{R\text{-}EF}$ and $Te_{R\text{-}SD}$	$G_{R\text{-}EF}$ and $G_{R\text{-}SD}$
1	Measured/ calculated and verified	The data (collection date) can be maximum 2 years old with respect to the "reference year" of the dataset	The "reference year" of the tendered dataset falls within the time validity of the secondary dataset	Technology aspects have been modeled exactly as described in the title and metadata, without any significant need for improvement	The processes included in the dataset are fully representative for the geography stated in the "location" indicated in the metadata
2	Measured/ calculated/ literature and plausibility checked by a reviewer	The data (collection date) can be maximum 4 years old with respect to the "reference year" of the dataset	The "reference year" of the tendered dataset is maximum 2 years beyond the time validity of the secondary dataset	Technology aspects are very similar to what described in the title and metadata with need for limited improvements. For example, use of generic technologies' data instead of modeling all the single plants.	The processes included in the dataset are well representative for the geography stated in the "location" indicated in the metadata
3	Measured/ calculated/ literature and plausibility not checked by a reviewer OR qualified estimate based on calculations plausibility checked by a reviewer	The data (collection date) can be maximum 6 years old with respect to the "reference year" of the dataset	The "reference year" of the tendered dataset is maximum 3 years beyond the time validity of the secondary dataset	Technology aspects are similar to what is described in the title and metadata but merits improvements. Some of the relevant processes are not modeled with specific data but using proxies	The processes included in the dataset are sufficiently representative for the geography stated in the ""location" indicated in the metadata. E.g., the represented country differs but has a very similar electricity grid mix profile

(continued)

Table 5.2 (continued)

Score	P_{EF} and P_{AD}	$Ti_{R\text{-}EF}$ and $Ti_{R\text{-}AD}$	$Ti_{R\text{-}SD}$	$Te_{R\text{-}EF}$ and $Te_{R\text{-}SD}$	$G_{R\text{-}EF}$ and $G_{R\text{-}SD}$
4	Qualified estimate based on calculations, plausibility not checked by reviewer	The data (collection date) can be maximum 8 years old with respect to the "reference year" of the dataset	The "reference year" of the tendered dataset is maximum 4 years beyond the time validity of the secondary dataset	Technology aspects are different from what described in the title and metadata. Requires major improvements	The processes included in the dataset are only partly representative for the geography stated in the "location" indicated in the metadata. E.g., the represented country differs and has a substantially different electricity grid mix profile
5	Rough estimate with known deficits	The data (collection date) is older than 8 years with respect to the "reference year" of the dataset	The "reference year" of the tendered dataset is more than 4 years beyond the time validity of the secondary dataset	Technology aspects are completely different from what described in the title and metadata. Substantial improvement is necessary	The processes included in the dataset are not representative for the geography stated in the "location" indicated in the metadata

Abbreviations used in the indices: *EF* elementary flow, *AD* activity data, *SD* secondary data

The DQR of […] datasets shall be calculated as following:

1. Select the most relevant sub-processes and direct elementary flows that account for at least 80% of the total environmental impact of the company-specific dataset, listing them from the most contributing to the least contributing one
2. Calculate the DQR criteria Te_R, Ti_R, G_R and P for each most relevant process and each most relevant direct elementary flow.(…)

Afterward, the results for each of these "most relevant" elements are weighted according to the contribution of the overall impacts, yielding a DQR for one developed process as combination of the results for contributing processes (via products) and elementary flows. The Te_R, Ti_R, G_R, and P to be included in the formula above are weighted averages. Worth noting is that for processes, the formula is to be applied only for the EF-compliant datasets according to the PEFCR 6.3 (European Commission 2018a, p. 177), but the contribution of the non-EF compliant dataset to the 80% overall impact in percent is added to 1, and the DQR obtained from the formula, considering EF compliant datasets, is multiplied by a factor of 1 plus this relative contribution of the noncompliant datasets.

The procedure shows how difficult it is to come to a quantitative result for data quality; applying an equal weighting for each of the data quality indicators is certainly debatable, and even more, it seems not really specified how to arrive at data quality indicator results for an overall life cycle result, i.e., for aggregated processes.

The definition "most relevant" depends a lot on the LCIA method; a change in characterization factors may change what is considered most relevant for a product system. For precision, finally, a reviewer helps to increase precision; a qualified estimate without plausibility check by a reviewer is seen as less precise as the same estimate with plausibility check, independent of the position of the reviewer.

Review in the Environmental Footprint

A review is used in the EF to verify or validate various statements regarding compliance and data quality and can be seen as an essential part of the EF. Some of the points requiring a review in the EF include:

– Verification of data used in process datasets (see Sect. 3.5.1.2) the verification has an influence on the DQR rating
– Review of compliance with the PEFCR

Regarding the review procedure and reviewer qualifications, the EF relies on the ILCD review specifications (European Commission 2010), including reviewer qualifications and also review workflows.

3.5.2 Data Quality in the US Environmental Protection Agency

For the US Environmental Protection Agency (EPA), a guidance document for data quality in LCI has recently been published (Edelen and Ingwersen 2016). The data quality system distinguishes flows, processes, and (life cycle) models as main elements to be addressed. Five indicators are considered: time, geography, technology, and completeness constitute the representativeness of an element (i.e., flow, process, or model). They are seen as "dynamic" data quality indicators since they depend on the goal and scope setting for the element. As additional indicator "reliability" is considered, which is in contrast to the other four indicators seen as a static indicator that is not affected by a different goal and scope (Edelen and Ingwersen 2016); assuming that any LCA model always aims for reliable information, makes a different goal and scope unlikely.

For the indicators, a matrix is proposed, for flows and for the entire process dataset separately (Tables 5.3 and 5.4).

For the process level, only two indicators are considered (Table 5.4): One indicator to evaluate whether and how the process is reviewed; the other indicator to reflect how complete the process data set is.

Table 5.3 Data quality matrix for flows, US EPA

Indicator		1	2	3	4	5 (default)
Flow reliability		Verified data based on measurements	Verified data based on a calculation or non-verified data based on measurements	Non-verified data based on a calculation	Documented estimate	Undocumented estimate
Flow Representativeness	**Temporal correlation**	Less than 3 years of difference	Less than 6 years of difference	Less than 10 years of difference	Less than 15 years of difference	Age of data unknown or more than 15 years
	Geographical correlation	Data from same resolution **and** same area of study	Within one level of resolution **and** a related area of study	Within two levels of resolution **and** a related area of study	Outside of two levels of resolution **but** a related area of study	From a different or unknown area of study
	Technological correlation	All technology categories are equivalent	**Three** of the technology categories are equivalent	**Two** of the technology categories are equivalent	**One** of the technology categories is equivalent	**None** of the technology categories are equivalent
	Data collection methods	Representative data from >80% of the relevant market, over an adequate period[a]	Representative data from 60–79% of the relevant market, over an adequate period **or** representative data from >80% of the relevant market, over a shorter period of time	Representative data from 40–59% of the relevant market, over an adequate period **or** representative data from 60–79% of the relevant market, over a shorter period of time	Representative data from <40% of the relevant market, over an adequate period of time **or** representative data from 40–59% of the relevant market, over a shorter period of time	Unknown **or** data from a small number of sites **and** from shorter periods

Edelen and Ingwersen (2016, p. 8)

[a]Technology categories are process design, operating conditions, material quality, and process scale

Table 5.4 Data quality matrix for process datasets, US EPA

Indicator	1	2	3	4	5 (default)
Process review	Documented reviews by a minimum of two types[a] of third party reviewers	Documented reviews by a minimum of two types of reviewers, with one being a third party	Documented review by a third party reviewer	Documented review by an internal reviewer	No documented review
Process completeness	>80% of determined flows have been evaluated and given a value	60–79% of determined flows have been evaluated and given a value	40–59% of determined flows have been evaluated and given a value	<40% of determined flows have been evaluated and given a value	Process completeness not scored

Edelen and Ingwersen (2016, p. 9)
[a]Types are defined as either industry or LCA experts

Similar as for the EF, 1 is the best and 5 is the worst indicator value. A review does not have the role to provide assessment scores, but having a review is seen as a positive aspect directly. For the completeness assessment, a multistep procedure is proposed, where the dataset is evaluated per anticipated flow category.

The EPA guidance stresses the importance of documentation; it does not provide a default procedure for aggregating the different indicators, but instead leaves this at the discretion of every LCA practitioner (Edelen and Ingwersen 2016, p. 9).

3.5.3 UNEP Global Life Cycle Access to Data (GLAD)

The GLAD Access Network is an initiative by the United Nations Environment Programme and the Society of Environmental Toxicology and Chemistry (UNEP/SETAC) Life Cycle Initiative. It was founded in 2014 and is led by a steering committee that reports to a UNEP-hosted secretariat (UNEP/SETAC 2014). Guiding principles of GLAD are

(i) Access to LCA data is the prerequisite for scientifically sound LCA modeling
(ii) Only standardized LCA modeling under use of consistent datasets and established scientific methods can support policy-makers in pursuing the Sustainable Development Goals (SDG) 12 Responsible Production and Consumption (United Nations 2017)

GLAD's self-proclaimed vision is "a global network comprised of independently-operated and interoperable LCA databases that connects multiple data sources to support life cycle assessment in a way that facilitates sustainability-related decisions" (Hauschild et al. 2018).

As a result, different nomenclatures, different data formats, and different modeling approaches are "permitted" in GLAD, in addition to the common time, geography, and location indicators for data quality. At present, the indicators in Table 5.5 are specified and implemented in a search engine to access various datasets. At the GLAD website (https://www.globallcadataaccess.org/api.html), the table there presents metadata descriptors as addressed by the Application Programming Interface (API), see Table 5.5.

A broader public test with more data is in preparation. In comparison with other data quality assessments, GLAD tries to address differences in LCI modeling, which is a challenge since modeling aspects are more diverse than time or location. GLAD thereby has a distinctly different approach to data quality. It promises to indeed overcome modeling "silos," to increase data availability, and is the first to take the ISO definition of data quality serious, in that data quality is application dependent. This promises a more realistic treatment of fitness for purpose, to better allow users to really find the data that are needed, instead of a "one size fits all" approach where it is preempted what users need.

Table 5.5 GLAD metadata descriptors as addressed by the Application Programming Interface (API) for the GLAD website

API field	fieldformat	fieldcontent	default
refId:	string	The unique identifier of the data set *required	
name:	string	The name of the data set *required	
dataSetUrl:	string	A url to download the complete data set *required	
category:	string	The category of the data set. The value will be automatically built from the elements in the 'categories' field, concatenated with a slash (/). e.g. categories = ['Emission to air', 'Unspecified'] => category = 'Emission to air/Unspecified'	
description:	string	The description of the data set	
technology:	string	A description of the technology used in the data set	
format:	string	Enum:ECOSPOLD1, ECOSPOLD2, ILCD, JSON-LD, OTHER, UNKNOWN	
location:	string	The location of the data set	
dataprovider:	string	The name of the provider of the data set	
supportedNomenclatures:	string	The nomenclatures the data set is compliant to	
lciaMethods:	[string]	A list of supported LCIA methods	
categoryPaths:	[string]	(Internally) used to build a tree like category structure. This value will be automatically calculated from the elements in the 'categories' field. e.g. categories = ['Emission to air', 'Unspecified'] =>categoryPaths = ['Emission to air', 'Emission to air/Unspecified']	
unspscPaths:	[string]	(Internally) used to build a tree like structure for the unspsc code. This value will be automatically calculated from the 'unspscCode' field. e.g. unspscCode = '50454302' =>unspscPaths = ['50', '5045', '504543', '50454302']	
co2pePaths:	[string]	(Internally) used to build a tree like structure for the co2pe code. This value will be automatically calculated from the 'co2peCode' field. e.g. co2peCode = '1.1.1' => co2pePaths = ['1', '1.1', '1.1.1']	
processType:	string	Enum:UNIT, PARTIALLY_AGGREGATED,	Default: UNKNOWN

(continued)

Table 5.5 (continued)

API field	fieldformat	fieldcontent	default
		FULLY_AGGREGATED, BRIDGE, UNKNOWN	
representativenessType:	string	Enum:SCIENTIFIC, EXPERT_BASED	Default: EXPERT_BASED
modelingType:	string	Enum:ATTRIBUTIONAL, CONSEQUENTIAL, UNKNOWN	Default: UNKNOWN
multifunctionalModeling:	string	Enum:PHYSICAL, ECONOMIC, CAUSAL, SYSTEM_EXPANSION, NONE, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
biogenicCarbonModeling:	string	Enum:OMITTED, DISTINGUISHED, AGGREGATED, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
endOfLifeModeling:	string	Enum:CUT_OFF, PHYSICAL_APOS, ECONOMIC_APOS, SUBSTITUTION, OTHER, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
waterModeling:	string	Enum:AMOUNTS, AMOUNTS_AND_AVAILABILITY, AMOUNTS_AND_QUALITY, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
infrastructureModeling:	string	Enum:INCLUDED_AND_DISTINGUISHED, INCLUDED_AND_NOT_VISIBLE, NOT_INCLUDED, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
emissionModeling[11]:	string	Enum:INCLUDED_AND_DISTINGUISHED, INCLUDED_AND_NOT_VISIBLE, NOT_INCLUDED, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
carbonStorageModeling:	string	Enum:INCLUDED_AND_DISTINGUISHED_CORRECTION, INCLUDED_AND_DISTINGUISHED_OTHER, INCLUDED_AND_NOT_VISIBLE, NOT_INCLUDED, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
sourceReliability:	string	Enum:MEASURED_VERIFIED, PARTLY_MEASURED_VERIFIED, PARTLY_MEASURED_PARTLY_ESTIMATED, ESTIMATED_QUALIFIED, ESTIMATED_UNQUALIFIED	Default: ESTIMATED_UNQUALIFIED
aggregationType:	string	Enum:HORIZONTAL, VERTICAL, COMBINED, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
reviewType:	string	Enum:INTERNAL, EXTERNAL, PANEL, UNKNOWN, NONE	Default: NONE
reviewSystem:	string	Enum:ILCD, PEF, GHG, LCA_UN, OTHER, UNKNOWN, NOT_APPLICABLE	Default: NOT_APPLICABLE
unspscCode:	string	A UNSPSC process code categorizing the data set	
co2peCode:	string	A CO2PE product code identifying the product of the data set	
copyrightHolder:	string	The owner of the copyright of the data set if applicable	
license:	string	The license the data set is released under	
contact:	string	A contact person for infomation on the data set	
categories:	[string]	The categories of the data set as array (one entry per child category)	
reviewers:	[string]	A list of the names of the reviewers of the data set	
validFrom:	integer (int64)	The start of the validity of the data set in milliseconds since 01/01/1970 (unix-time tims 1000)	
validUntil:	integer (int64)	The end of the validity of the data set in milliseconds since 01/01/1970 (unix-time tims 1000)	
validFromYear:	integer (int32)	The year of the start of the validity of the data set, will be taken from validFrom if not set	
validUntilYear:	integer (int32)	The year of the end of the validity of the data set, will be taken from validUntil if not set	
latitude:	number (double)	The latitude of the geography of the data set	
longitude:	number (double)	The longitude of the geography of the data set	
completeness:	number (double)	The percentage of flows according to nomenclature	Default: 100
amountDeviation:	number (double)	The deviation in mass and energy balance	
representativenessValue:	number (double)	The percentage of variation coefficient, s/(arithm mean)	
copyrightProtected:	boolean	Indicates if the data set is copyright protected	
free:	boolean	Indicates if the data set is available for free	
publiclyAccessible:	boolean	Indicates if the data set can be downloaded from the given dataSetUrl without further login	

[a]Meant for addressing long-term emissions

4 Notes on Selected Data Quality Indicators

While different frameworks may use different indicators to reflect fitness for purpose and data quality, some indicators are commonly used, sometimes with slightly deviating meaning, and have been present in discussions of data quality since early on. They are presented and discussed in the following sections.

4.1 Uncertainty

Instead of uncertainty, the absence of certainty for a value or something else, also "precision" is used sometimes as antonym, and "imprecision" as synonym. ISO 14040 distinguishes model imprecision, input uncertainty, and data variability (ISO 14040, 3.33). Model imprecision refers to modeling decisions that are, from one LCA modeler to another or from one modeler over time, not fully identical, and thus not certain (choice of system boundaries, of allocation rules, etc.). Input uncertainty refers to input data in an LCA model that is not fully certain, typically because it is not fully known (for example, a specific type of fertilizer with a specific supply chain is not known, instead a generic fertilizer is used). This type of uncertainty is also called "parameter uncertainty" (Huijbregts 1998). "Variability" refers to occurrences that change in reality but are not reflected in an LCA model (Huijbregts 1998); an example is changed water demand of perennial crops over the year.

For an LCA model, a result with high uncertainty is not desirable, independent from the application of the LCA model, be it "accounting" (i.e., a mere report on impact figures linked to a product system) or, more frequently, decision-support. That said, it is very positive if an LCA model, i.e., a process dataset or a product system result, reports the uncertainty of its quantitative amounts. This reporting can be an ordinal uncertainty class (low uncertainty, higher uncertainty) or also a full quantitative uncertainty, with ranges or probability distribution functions.

Regarding quantitative uncertainty, typically a relative value is more interesting than an absolute one, since the absolute amount depends on the choice of the unit. Uncertainty appears in the PEF data quality system as "precision" and addresses reliability of the source, implying reliability of the result (see Sect. 3.5.1). For the GaBi databases, the indicator precision is used, and assessed based on the reliability of the source ("measured" gets best score, then "literature," "calculated," and "estimated"). Interestingly, the uncertainty of data is seen as almost least important by the GaBi database; the only provision of unit processes is less important, but the precision of data is seen as much more important (Fig. 5.5).

In ecoinvent, quantitative probability distribution function results are provided based on data quality indicator ordinal scores, which are combined with expert guesses. To some extent, this is explained in Ciroth et al. (2013), and especially because the original values from ecoinvent which "transform" indicator scores into quantitative uncertainty are not documented, which raises doubts and questions regarding the provided quantitative uncertainty figures. In the GLAD system,

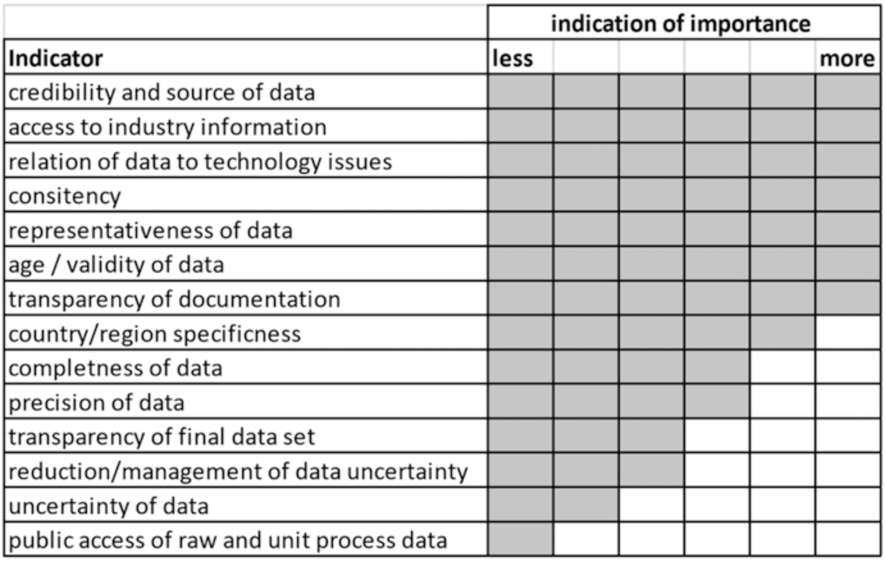

Fig. 5.5 Qualitative importance of data quality aspects and indicators in GaBi databases (Kupfer et al. 2017, p. 76), screenshot from the source

uncertainty is not addressed as an indicator. In the US EPA system, uncertainty is not part of the data quality indicators.

Uncertainty typically propagates through an LCA model (Ciroth et al. 2004). It is somewhat speculative to estimate uncertainty without further qualification, as would be usually needed for aggregated process uncertainty. As a consequence, most databases do not report uncertainty for aggregated processes.

The LCA world is far from agreeing on how to deal with uncertainty in the inventory and in datasets. Uncertainty in LCA today suffers from a lack of empirically-based data. Uncertainty is often not reported and there are very few cases where it is addressed in primary data collection.

While the "direction" of the uncertainty indicator is always the same, with less uncertainty being better, the accepted level of uncertainty can depend on the application. More far-reaching decisions will typically require a lower uncertainty. However, since the overall uncertainty modeling in LCA is not too far developed and empirical uncertainty is typically not available, there exist today only expert guesses on the acceptable level of uncertainty in use.

4.2 Reliability

Reliability in LCA data quality typically refers to the reliability of the *source* to address that some information sources in LCA are more reliable than others. A more reliable source is always desirable, independent from the application. Sources are typically ordered in reliability classes in different LCA data quality systems, with almost identical results. Independently peer-reviewed, empirical-based sources are seen as most reliable, unqualified estimates as least reliable (Weidema et al. 2013).

A reliable source can also report that some information is not reliable, for example, that a short measurement was performed on a small sample, which might lead to a high uncertainty. If these measurement results are verified, we have a very reliable source (empirical measurement with results verified), where, however, the result is not fully reliable, due to the small sample.

Recently published data quality systems sometimes "shortcut" reliability of the source with *reliability of the result*, in that a reliable source automatically creates reliable results. This might not be true, as the simple example above illustrates.

An example is the indicator "flow reliability" in the US EPA system (see Sect. 3.5.2): a measured and verified result for a flow scores best in reliability. For the EF system, reliability is, somewhat surprisingly, mixed with precision, thereby implying that a reliable source always leads to precise results. This excludes variability from precision, since variability cannot be controlled and thus might lead to imprecise results even for a reliable source.

Specific applications can require specific data sources, but typically this rather refers to specific background databases than to reliable classes of information. An example is Environmental Product Declarations and the EF; in EF-compliant LCA models, the tendered background datasets are required to be used as a background database (European Commission 2018a).

4.3 Representativeness

Representativeness is an interesting data quality indicator in LCA. It addresses whether and how much a given information is able to represent a larger group, i.e., serve as a typical or characteristic example.[10] Representativeness is commonly used in statistics; in other words, information can be considered representative (only) if the information is obtained by random sampling, i.e., a sampling where all items of interest, called "population" in statistics, have a known chance of being drawn (e.g., Hansen et al. 1953, Vol I p. 9[11]). Random sampling is very uncommon in LCI, and often simply rejected because of practical limitations (it is hardly possible to include all German milk farmers in one study and draw randomly those farmers from where more detailed data is collected). However, there are some examples of statistical sampling in LCA; so it was possible to determine the fully representative weight of a 150 g yogurt cup sold in Berlin, by sampling from supermarkets (Ciroth and Srocka 2008; Fig. 5.6).

[10] https://www.merriam-webster.com/dictionary/representative

[11] Who continues: "When the determination of the [items] included in a sample involves personal judgement, one cannot have an objective measure of the reliability of the sample results, because the various [items] may have differing and unknown chances of being drawn." (Hansen et al. 1953, Vol I p. 9.)

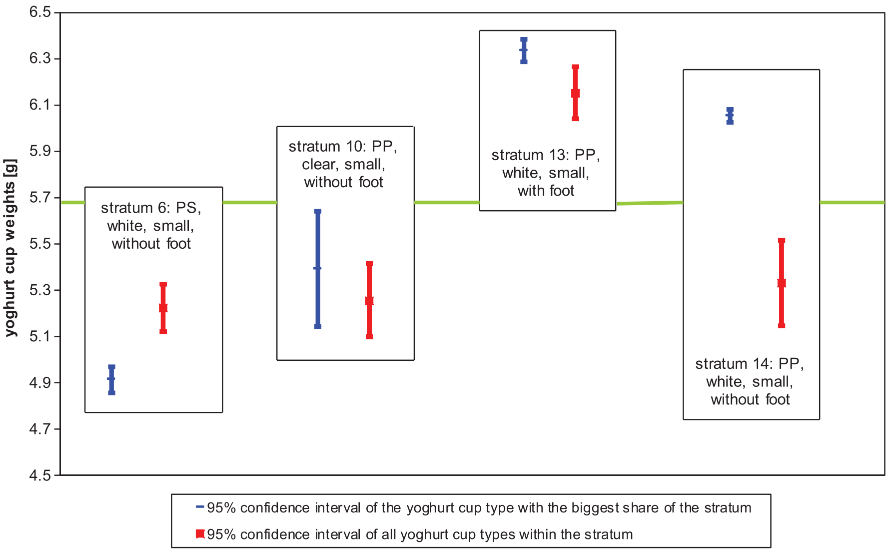

Fig. 5.6 Weight of different types of yogurt cups sold in supermarkets in Berlin, market leader and representative market average (Ciroth and Srocka 2008)

In the US EPA system, representativeness refers in a wider sense to how well a dataset represents time, location, and technology of the targeted dataset; these three indicators will be discussed in Sects. 4.4, 4.5, and 4.6. In a more narrow sense, representativeness refers to how representative the dataset is (see Table 5.3), by considering the share of data that is representative for a given and stated market. “Representative” itself is not further defined in the source, however. For the PEF, representativeness is a central aspect. The PEF pilots aim to provide results for representative products; the category rules that determine the details of the models for each product category can be considered representative of a certain product category if (i) main competitors have been invited with at least 75% market coverage, (ii) stakeholders participating in the process of developing the category rules cover at least 51% of the market, and (iii) “a wide range of stakeholders” have been invited for the discussion process, including Small and Medium Enterprises (SMEs), by the Technical Secretariat[12] (European Commission 2018a, p. 31). Market share is used as a proxy for representativeness here.

Previous data quality assessment frameworks for LCA used market share directly as a proxy for representativeness, which contrasts to findings from statistical science and sampling; it often occurs that market leaders are significantly different from smaller market competitors, thus a high market share alone might lead to biased results.

[12] The Technical Secretariat is responsible for steering the whole process of PEFCR development for a specific product category.

The approaches of both the PEF and the US EPA seem to recognize this, but do not provide means for addressing representativeness in a statistical, science-based way.

4.4 Time

Time is a data quality indicator considered since the very first data quality deliberations in LCA. A dataset represents a certain time frame, i.e., it is meant to be valid for this time. With time passing, input and output flows of a process can change, for a variety of reasons, so different weather conditions (heating, agricultural processes), technological changes, or also legal changes. Depending on the technology and also on the specific flow in a process dataset, changes happen slower or faster. Figure 5.7 shows changes in European car emissions to the air from the HBEFA[13] database over the years 1990–2010, per person-km; while all pollutants change to some extent; emissions of lead and of sulfur dioxide change drastically; for sulfur dioxide, the geometric standard deviation increases by a factor of about 3.5, especially from 1990 until 2005, for lead by a factor of 1.75 from 1990 to 1995. The change in lead emissions can be explained by the introduction of catalyst cars and the reduction of lead content in fuel; with EN 590:1993 and EN 228:1993, a first threshold for sulfur content was introduced in October 1994, and the threshold was further lowered in several steps with the enforcement of the various Euro emission

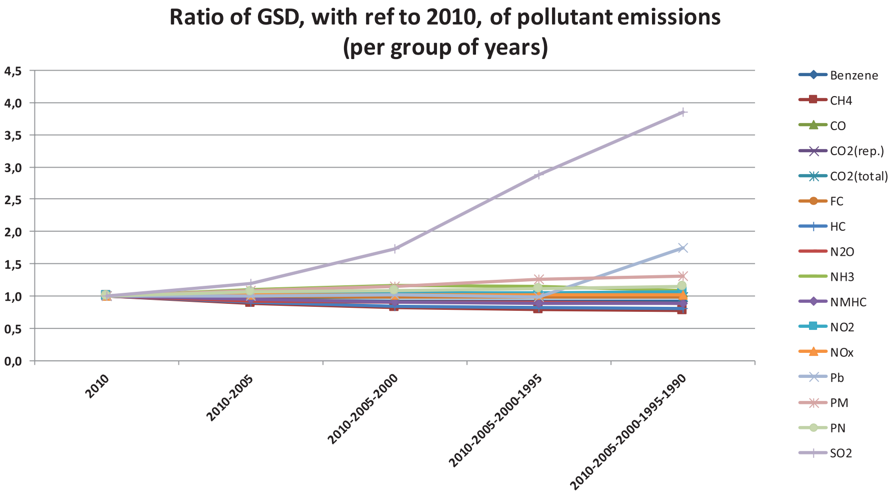

Fig. 5.7 Changes of different car emissions, European average passenger car, for 2010 and a wider range of years; geometric standard deviation (GSD) of the sample with 2010 as reference, following (Ciroth et al. 2013)

[13]The Handbook Emission Factors for Road Transport, http://www.hbefa.net/e/index.html

standards, from 2000 ppm to 10 ppm with Euro 5, implemented 2009.[14] This evidently has a direct effect on sulfur dioxide emissions, since sulfur in fuel is oxidized in fuel combustion and typically releases as sulfur dioxide.

4.5 Location

Location has potentially quite a large influence on inventory processes, albeit for some processes more than for others. Influence may come from differing applicable legislation, such as banning of ingredients in food, of certain chemicals, and of pest control measures (van den Berg et al. 2017). It may also come from different climatic conditions and conventions, which might influence heating and cooling in buildings (Ürge-Vorsatz et al. 2015) as well as agricultural processes. Available nutrients in the soil, available water, temperature, and other climatic conditions often determine the type of crop and influence yield, the need for irrigation, pest control fertilizers, and in-field operations for the same type of crop grown at different locations.

Table 5.6 shows differences in cotton yield worldwide, with a ratio between Pakistan and Australia of about 2.6.[15]

4.6 Technology

Technology refers to the product and the production process; it is probably the one data quality indicator that most determines the specific inventory of a process dataset. Commonly, the indicator used in data quality frameworks is called "further" technological representation, meaning that this indicator addresses differences that are not considered by the other indicators: time, location, and also other indicators may impact the technology used in the process as well.

The US EPA data quality framework distinguishes process design, operating conditions, material quality, and process scale as categories of technological representation, obviously with the idea that e.g., a different process scale has the chance to change the process entirely; in GLAD, UNSPSC[16] category "distance" is used as an indicator for technical difference. In the EF, the technology indicator is somewhat vaguely described.

For example, for score 3, the criterion says: "*Technology aspects are similar to what described in the title and metadata but merits improvements. Some of the*

[14] https://www.transportpolicy.net/standard/eu-fuels-diesel-and-gasoline/

[15] Source: Foreign Agricultural Service, Official USDA Estimates, https://apps.fas.usda.gov/psdonline/app/index.html#/app/advQuery

[16] The United Nations Standard Products and Services Code, https://www.unspsc.org/

Table 5.6 Cotton yield in kg/ha for different countries worldwide, for the year 2018/2019

Country	Yields 2018/2019	Unit Description
Pakistan	698.54	(kg/ha)
Iran	704.41	(kg/ha)
Egypt	750.78	(kg/ha)
United States	939.46	(kg/ha)
Colombia	967.67	(kg/ha)
Spain	1004.89	(kg/ha)
Peru	1024.60	(kg/ha)
South Africa	1040.25	(kg/ha)
Bulgaria	1088.63	(kg/ha)
Tunisia	1088.63	(kg/ha)
Syria	1132.18	(kg/ha)
Kyrgyzstan	1143.06	(kg/ha)
Venezuela	1233.78	(kg/ha)
Greece	1253.04	(kg/ha)
Turkey	1549.21	(kg/ha)
Mexico	1578.06	(kg/ha)
Israel	1632.95	(kg/ha)
Brazil	1636.42	(kg/ha)
China	1726.26	(kg/ha)
Australia	1814.39	(kg/ha)

Table 5.7 Examples for the various scores for the indicator "further technological representation" Ciroth et al. (2012, p. 45)

Indicator score	Meaning of the indicator score	Differences in datasets relevant for this indicator score
1	Data from enterprises, processes, and materials under study	Personal car, EURO 4 emission type, 1.4–2 l capacity, inner city use, diesel
2	Data from processes and materials under study (i.e., identical technology) but from different enterprises	For personal car: Different use, inner city use versus other use types
3	Data from processes and materials under study but from different technology	For personal car: Different size (0–1.4 l, 2–9 l), different emission category (EURO 1, 2, 3, and 5 in addition to 4)
4	Data on related processes or materials	For personal car: Also old cars (pre Euro 1)
5	Data on related processes on laboratory scale or from different technology	For personal car: Different fuel (gasoline)

relevant processes are not modelled with specific data but using proxies." This leaves space for interpretation: what does exactly "similar" mean; what are relevant processes for background datasets? Table 5.7 shows some examples for indicator scores to address technological representation.

5 Conclusion and Way Forward

Data quality is at the core of LCA modeling and of providing relevant LCI databases. ISO 14040 defines data quality as "fitness for purpose" and thereby makes data quality application-(or purpose-)dependent. This is challenging for LCI databases with regard to their claim that their datasets are of high quality, and it is even more challenging when users want to combine datasets from different, quality-assured databases.

The recent project GLAD, initiated by UNEP, has first developed a more comprehensive view on data quality, where also modeling aspects are addressed. This system promises to better address data quality also across different databases and for a variety of applications, but so far is waiting for a broader implementation.

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Chapter 6
Life Cycle Inventory Data and Databases

Andreas Ciroth and Salwa Burhan

Abstract Life cycle inventory (LCI) databases are commonly used in life cycle assessment (LCA) studies. They enable modern, larger case studies, make data collection more efficient, and help to establish comparability across different case studies. A database typically tries to provide one coherent and consistent modeling space, thereby allowing users to take different datasets in the appropriate database, which implies that the goal and scope of datasets in the database match the goal and scope of case studies done with the database.

This chapter explains the principal elements of LCI data, different types of databases in LCA, and explores common issues in modern LCA databases: starting a database, maintaining it, providing quality assurance, and not the least, making the database available to users. The second part of the chapter deals with data exchange and data exchange formats, as well as with interoperability concepts to allow the use of datasets from different databases in one study.

Keywords Background system · Data exchange formats · Data exchange · ELCD (European Reference life cycle database) · Elements of LCA data · Environmental footprint · Fitness for purpose · Foreground system · GLAD (Global Life Cycle Access to Data) · Harmonized data sets · Interoperability · LCI data · LCI databases · Life cycle assessment (LCA) · Life cycle impact assessment (LCIA) methods · Life cycle inventories (LCI) · ProBas (LCI library from the German Environmental Protection Agency) · Unified modeling language (UML) · US EPA (US Environmental Protection Agency)

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1 Life Cycle Inventory Data and Databases, Definition and Introduction

As introduced in Chaps. 1[1] and 3[2] in this book, a life cycle inventory is a model of the life cycle of a product or service, with quantified inputs and outputs, and thereby comprises processes, flows, and units. When translating this into an IT model, flow properties such as mass or energy may be added, and the entire life cycle model may be called a product system, as a model of the connected processes.

Figure 6.1 shows an example from an early version of the openLCA software, where the main elements of inventory data are shown with their relations, using unified modeling language (UML) notation.

A process (dataset) is linked to one or many actors (authors, reviewers, distributors, and so forth), can contain references to one or many flows, and link to one or many sources; a flow links to one or many flow properties. A flow property refers to exactly one unit group (mass; unit groups of mass, containing, e.g., kilogram as one unit). Strictly speaking not part of the inventory are obviously life cycle impact assessment (LCIA) methods, where each method links to at least one flow. On a higher modeling level, there are product systems as structured collections of processes; one product system can contain one or several processes. Projects as comparisons of product systems are not common to all LCA data structures but they exist; evidently, then, one project contains one or more product systems.

All the elements in Fig. 6.1, apart from the LCIA methods, belong to the inventory. Therefore, all data found in and provided by these elements are inventory data.

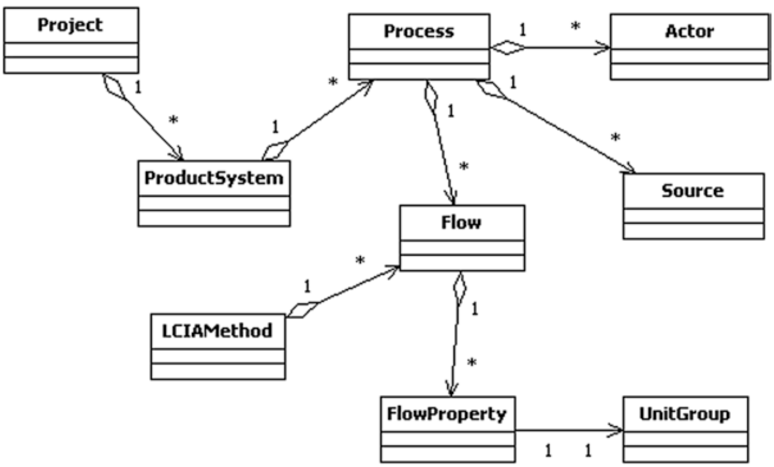

Fig. 6.1 Structure of main elements in LCA (Srocka 2009)

[1] Introduction to "Life Cycle Inventory Analysis"

[2] Development of Unit Process Datasets

Some of the elements, like the flow properties, are rather simple and do not contain a lot of more detailed information. Others, such as the process data set, are more complex and may contain, depending on the specific database or exchange format, hundreds of sub-elements, including flows with exchanges and direction, amount and unit, as well as metadata with modeling details.

A life cycle inventory (LCI) database can be defined as (UNEP/SETAC 2011, p 137):

> A system intended to organize, store, and retrieve large amounts of digital LCI datasets easily. It consists of an organized collection of LCI datasets that completely or partially conforms to a common set of criteria, including methodology, format, review, and nomenclature, and that allows for interconnection of individual datasets that can be specified for use with identified impact assessment methods in application of life cycle assessments and life cycle impact assessments.

The main distinction from a dataset library is the intent to provide harmonized process datasets which can be easily and without major mistakes used together, for the creation of LCA and LCIA models and for calculating them.[3] The definition recognizes that the attempt to provide such a harmonized, "safe" space is often not fully possible.

One of the largest, global attempts for the harmonization of process datasets and databases "culminated" in a workshop on Global Guidance Principles for Life Cycle Assessment Databases, held in Shonan, Japan in 2011, after longer preparation. These guidance principles, commonly called the "Shonan Guidance Principles," focused on principles for creating, managing, and disseminating datasets to aid life cycle assessments of products and services globally (UNEP/SETAC 2011).

2 The Role of Life Cycle Inventory Databases for Life Cycle Assessment

The first LCA case studies consisted of about 50 processes, which were meant to reflect the entire life cycle (Gilgen et al. 1994; UBA 1995). This holds also for recent social LCA case studies (Ciroth and Franze 2011). These studies often took years to finish. In comparison, recent case studies contain hundreds to thousands of process data sets, and typically take less time and effort. This is only possible because of LCI databases available and in use for these case studies. Most of the processes are not generally modeled in the project but instead taken from the LCA databases.

Commonly, LCA studies are then distinguished into a foreground and a background system (Frischknecht 1998); the foreground system reflects the specific

[3] We implicitly define LCI data library here; in an LCI library, the provider of the datasets does not attempt to harmonize them, for example, to preserve the original modeling of the datasets. A "classic" example of an LCI library is ProBas, from the German Environmental Protection Agency, http://probas.umweltbundesamt.de/

product under study, while the background system is completed by using data from generic LCA databases.

This is more efficient than modeling common processes such as electricity and transport from the bottom up each time. It ensures consistency among practitioners that are performing LCA studies using the same database, and it makes realistic case studies in reasonable time possible. Often, the main contribution of the impacts in an LCA case study comes from the generic database, i.e., the background system, which is then more important than the foreground system for impact results. This shows the relevance of LCI databases for LCA and points at the importance of background datasets matching the goal and scope of the study.

On the other hand, since each database tries to provide one consistent, "safe modeling space," this raises the question whether methodology and nomenclature of the database fit to methodology and nomenclature of the to-be-conducted study. Further, the unspecific, generic product provided in the database may not suit the specific product needed by the foreground system, which can be difficult for uncommon products (a specialty chemical, for example) or also for products from different regions (truck transport in India instead of truck transport in the European Union). Finally, different databases used in combination in one study may not fit together, as each of their "safe modeling spaces" might be inconsistent to each other, and the choice of one or the other database can have a strong influence on the overall result of a study. Some LCA studies performed a comparison between different LCI databases available for the building sector, where their methodology, documentation, data quality, and comprehensiveness were examined (Takano et al. 2014; Martínez-Rocamora et al. 2016). Based on their study, Takano et al. recommended enhanced information sharing between databases over developing newer databases. They also recommended the creation of a reporting and communication system for LCAs instead of trying to harmonize the methodologies among the databases.

Thus, nowadays professional, well-managed LCA databases seem essential for performing LCA case studies. They save time and effort and help to focus on specific, relevant aspects of the case study. On the other hand, the selected database can largely influence the modeled life cycle and calculated results in a case study. Therefore, providing and selecting a database for a study requires care.

3 Types of Databases

The first databases were created in the late 1980s and early 1990s. Meanwhile, more and more databases are appearing, and a market for LCA databases has been set up. A recent United Nations publication (Sonnemann et al. 2016, p. 56) lists about 40 different databases. As of today, after 3 years, only a handful databases have been updated, some new have emerged, and one major database was discontinued (Table 6.1).

Databases differ in various aspects. Some main aspects are mentioned here, with examples from Table 6.1:

Table 6.1 Overview of selected LCA databases and libraries, country of origin, as well as number of datasets in 2012 and 2019

Name	Country (of database creator)	Type (DB: database, L: library)	Number of datasets as of 2012 (version or version year, if available)	Number of datasets, as of 2019	Comment
AGRIBALYSE	France	Process (DB)	822 (v1.2)	1188 (v1.3)	Last updated in 2015. AGRIBALYSE v3.0 is in development.
Agri-Footprint	Netherlands	Process (DB)	–	6342 (v4)	With some identical datasets from ELCD in different allocation models.
Australian Life cycle Inventory Database (AUsLCI)	Australia	Process (DB)	> 150	> 460	Database updates are ongoing.
Banco Nacional de Inventarios do Ciclo de Vida (SICV)[g]	Brazil	Process (DB)	10	22	Database updates are ongoing.
BioEnergieDat	Germany	Process (DB)	178	178	Last updated in 2012. There is no new project for updating the database.
Canadian Raw Materials Database (CRMD)	Canada	Process (DB)	13	18 (?)	
Chinese Life Cycle Database (CLCD v0.8)	China	Process (DB)	600	600	Last updated in 2011.
Ecobase	Chile	Process (DB)	147	147	The EcoBase database creation was a 2 year project that ended in 2015.
ecoinvent v3	Switzerland	Process (DB)	11,302 (v3.1)	16,024 (v3.5)	
ELCD 3.0 (European Life Cycle Database)	EU	Process (DB)	334	–	ELCD has been discontinued since 29 June 2019.
Extensions of ecoinvent data v.2.2	Switzerland	Process (DB)	6841	6841	Ecoinvent has since published ecoinvent v3 databases, the latest being ecoinvent v3.5, published in 2018.

(continued)

Table 6.1 (continued)

Name	Country (of database creator)	Type (DB: database, L: library)	Number of datasets as of 2012 (version or version year, if available)	Number of datasets, as of 2019	Comment
GaBi LCA Databases 2019	Germany	Process (DB)	6513 (2013)	12,500 (2019)	Latest update available for 2019.
Inventory Database for environmental Analysis (IDEA)[d]	Japan	Process (DB)	3000 (v1)	3800(v2)	Last updated in 2016.
LCACommons[i]	USA	Process (DB)	–	9207	Subsuming the US LCI database.
LCADB.sudoe	Catalonia, Spain	Process (DB)	72	72	Last update unknown.
Mexicaniuh[h]	Mexico	Process (DB)	81	81	No known update.
MY-ILCD[b]	Malaysia	Process (DB)	160	181	The Malaysian LCI database is not freely available, with only limited access to metadata level information.
NEEDS	International	Process (DB)	187	187	Not updated anymore.
Ökobau.dat (2014–2019-I)[c]	Germany	Process (DB)	954 (v2014)	1183 (v2019-I)	The current version of Ökobau.dat is 2019-I from 27 Feb 2019.
PEF tendered background datasets[j]	EU	Process (DB)	–	3504	Available for free for use within PEF, 2019.
ProBas	Germany	Process (L)	>8000	> 8000	Last known update in 2015.
Quantis Water Database[f]	Switzerland	Process (DB)	4000	4000	Last known update in 2012. Not publicly available database.
Quebec LCI database	Quebec, Canada	Process (DB)	900	900	The project for creating the database ended in December 2013.
SPINE@CPM[a]	Sweden	Process (DB)	>740	748	The first project was majorly funded by VINNOVA, Sweden's innovation agency between 1996 and 2006. It has been updated intermittently.

(continued)

Table 6.1 (continued)

Name	Country (of database creator)	Type (DB: database, L: library)	Number of datasets as of 2012 (version or version year, if available)	Number of datasets, as of 2019	Comment
Thai National Life Cycle Database[e]	Thailand	Process (DB)	1300	1484	Last updated in 2017.
U.S. Life Cycle Inventory Database	USA	Process (DB)	880	880	Has become part of the LCACommons.
eora[k]	Global	IO (DB)	14,839	14,839	Time series for the database available, 1990–2015.
exiobase[l]	Global	IO (DB)	9600 (v2.2)	9800 (v3.4)	Time series for the database available, 1995–2011.

[a] http://cpmdatabase.cpm.chalmers.se/
[b] http://lcamalaysia.sirim.my/index.php/databases
[c] https://www.oekobaudat.de/en/database/database-oekobaudat.html
[d] http://idea-lca.com/?lang=en
[e] http://spaces.oneplanetnetwork.org/system/files/8b_database_roadmapping_key_considerations_thailand_11-17.pdf
[f] https://quantis-intl.com/tools/databases/quantis-water-database/
[g] http://sicv.acv.ibict.br/Node/processList.xhtml?stock=IBICT
[h] http://www.centroacv.mx/mexicaniuh.php
[i] http://www.lcacommons.gov/
[j] http://eplca.jrc.ec.europa.eu/LCDN/contactListEF.xhtml
[k] http://www.worldmrio.com/
[l] http://www.exiobase.eu/

– Databases may have a specific *regional scope*. They contain processes that represent a specific region. In part, this may be intentional or the result of practical limitations. For example, there are databases intentionally specific for one country (the Thai National database for Thailand, My-ILCD for Malaysia). There are databases intending to cover larger regions (ELCD, the European Reference life cycle database, for Europe), and databases with an intended global scope (ecoinvent, although originally started from Switzerland, with datasets from other regions being added over time; exiobase, with 49 countries and larger regions; eora, with overall 192 countries).
– Databases may have a *technical scope*, i.e., processes that represent specific technologies and provide certain products and services. As for the regional scope, there are databases that are intentionally broad and generic, and specific databases that focus on, for example, one industry sector. Quite a number of databases focus on agriculture (Agribalyse, Agrifootprint, ESU Worldfood), some on building components (ÖkobauDat). Other databases are intentionally generic/broad (GaBi professional, ecoinvent, exiobase, and eora). Similar to the regional coverage, the intended broad technological coverage can be more or less complete.

- Databases may differ in the *resolution of industrial activities* included. Roughly speaking, databases either report processes ("set of interrelated or interacting activities which transforms inputs into outputs," ISO/TS 14048 (ISO/TS 14048: 2002[4]) following ISO 9000) or sectors (so-called I/O databases based on public statistics). In Table 6.1, eora and exiobase are I/O databases, whereas the other databases are process-based. For the process-based databases, some provide unit processes (again as defined in ISO/TS 14048, see also Chap. 3 in this book[5]), some only (or in addition) aggregated processes, with full or partial aggregation
- For using the database, also *organizational and procurement* aspects play a role. Some databases are free, some for purchase, with costs up to more than €10,000 per single-user license. Some databases are provided by public institutions (LCACommons, ELCD), some by private operators. Databases are furthermore updated at varying frequency, see Table 6.1.
- Databases further differ in their *quality assurance*. Most databases perform a review, some also by using external support from independent reviewers. These follow different review workflows and review schemes.
- Databases may differ in mere *technical aspects*, for example, in the implemented or supported import/export interfaces, the distribution "channel" of the database, for example, as part of an LCA software or stand-alone (see Sect. 4.4).
- Since databases aim to provide one coherent, consistent modeling space, it is evident that the *LCA methodology* may differ between databases, given that one universally accepted modeling approach does not exist yet. As a consequence, databases differ in various LCA choices, such as system boundaries, ways to deal with multifunctional processes and end of life, modeling biogenic, carbon and long-term emissions, to name just some of the typical LCA choices. A notable example are the three different "system model" databases provided by ecoinvent, which differ in the way they address end of life, allocation, and system expansion as well as linking processes.
- A related aspect is the supported *nomenclature* of the database, especially the supported elementary flow reference lists and supported LCIA methods.
- Finally, databases may differ in the addressed different *sustainability dimensions*. They may provide environmental inventory data, LCIA data, cost data, or also data about social impacts, alone or in combination, or also information only about climate-related impacts.

The first LCA databases were released in Switzerland (ecoinvent), Scandinavia (Sweden with SPINE@CPM, Finland with KCL-ECO), Germany (GaBi), Japan (IDEA), and in the US (USLCI), with a typically local data coverage. Over time, databases have been published also for other parts of the world, with focus on more

[4] ISO/TS 14048 (2002) Environmental management – Life cycle assessment – Data documentation format. 1st ed Geneva, Switzerland. ISO/TS 14048 was prepared by Technical Committee ISO/TC 207 "Technical Management," Subcommittee SC 5 "Life Cycle Assessment" in 1993. This standard was last reviewed and confirmed in 2013, therefore the version of 2002 remains current

[5] Development of Unit Process Datasets

local processes and products (e.g., palm oil, (Archer et al. 2018), bananas, coffee, etc.), or different realizations of the same processes (truck transport in Brazil), often also linked to a capacity-building effort. One example is the recently concluded Sustainable Recycling Industries (SRI) initiative funded by the Swiss State Secretariat for Economic Affairs (SECO) in partnership with ecoinvent, where regional LCI networks (Brazil, Egypt, India, and South Africa) were set up to collaborate with the local networks for promoting capacity-building in developing LCI for the respective regions.[6]

The varying content of databases can be seen when plotting the number of datasets in a database per sector against the country. Using the same country names and the comprehensive UNSPSC[7] code for the sector classification, a plot of three databases that were all started with the idea to provide datasets as comprehensive and complete as possible shows major differences. Figure 6.2 shows an excerpt for the ELCD database, with countries in column A and UNSPSC sectors in line 2. Figure 6.3 shows the heatmaps for all compared databases, with dark background for better visibility. The ELCD database covers only a few sectors (mainly electricity, not readable of course from the plot) (a).The ecoinvent database v3.2 and 3.5 (band d) covers more sectors and has a focus on some countries, shown in the horizontal lines. The eora database has the most complete coverage of the three databases (c).

This short introduction shows the diversity of databases, which contrasts to the declared aim of database operators to create a "safe modeling space" for users, where datasets can be combined without major issues. The contrast comes evidently from that each single database that is in itself possibly consistent, but may not be

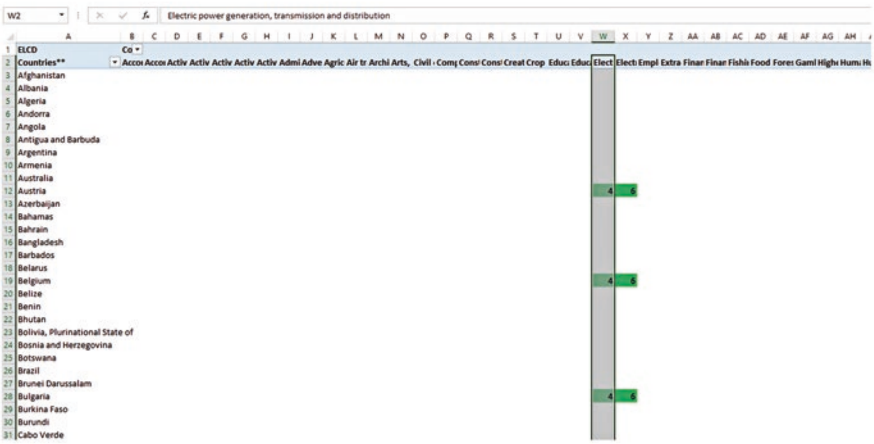

Fig. 6.2 Heatmap of the ELCD database, excerpt, countries, and sectors, with number of process datasets per sector in cells

[6] https://www.ecoinvent.org/about/projects/sri-project/sri-project.html

[7] The United Nations Standard Products and Services Code, http://www.unspsc.org/

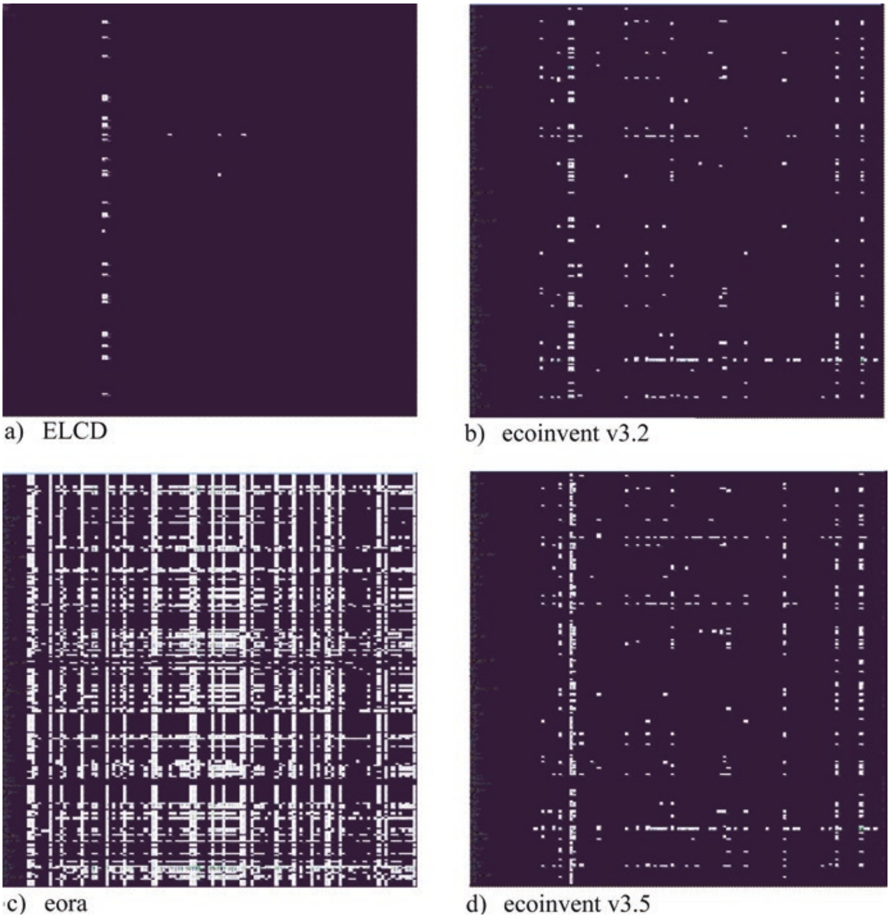

Fig. 6.3 Heatmap of different databases showing products and sectors (x axis) vs countries (y axis) covered

consistent compared to other databases; at the same time one single database may not be fully comprehensive so there is a need to reach across different databases. Therefore, for achieving a consistent space *across* different databases, three major approaches have emerged:

- The first approach is a network of consistent and aligned databases that promises to "expand" the harmonized data space and at the same time operate several databases independently. This idea was followed in the ILCD data network (JRC-IES 2010). Challenges in this solution are a harmonization of the datasets, i.e. to ensure that data sets are indeed aligned, as well as mere physical accessibility of the datasets, with sources of potentially varying reliability. A variant of this approach is an integration of a separately created database into one larger database, where the separately created database follows the modeling of the larger database. This was performed when the Quebecois's database was integrated into the ecoinvent database (Lesage and Samson 2016)

- A second approach is a mild harmonization of databases, concerning flow nomenclature and LCA-modeling related aspects, and the provision of all these databases in one central "repository." This is followed by the openLCA Nexus website[8] which is the largest repository of datasets available worldwide. An interactive map of the regionalized coverage of the datasets in the openLCA Nexus website is available in the Life Cycle Initiative website.[9] Obviously, a limitation is that processes in databases cannot be fully aligned; for system processes, mainly the nomenclature of flows can be changed, while the dataset modeling is "hidden" in the aggregation. Unit processes allow more changes, but an allocation applied to the process can be hardly changed, for example.

Both these options suffer from the limitation that they need to assume one specific modeling approach, flow nomenclature, and dataset use or set of uses, and try to apply this as consistently as possible. Possibly, the modeling approach is differentiated into several decision situations. For example, the ILCD handbook distinguishes decision support and accounting, and decision support with larger and small changes (ILCD Handbook 2010, pp. 38). This makes the database somewhat more flexible, but it still is unable to deal with many of the different modeling concepts and applications, which of course exist in "real-life" case studies.

Finally, as a further development, a system GLAD (see Chap. 5,[10] Sect. 3.5.3) was proposed and implemented in a first testing website (https://www.globallca-dataaccess.org/), through an international effort under the umbrella of UNEP/SETAC Life Cycle Initiative. The main idea is that several data providers submit datasets with "descriptors" that can be used to understand their modeling background and intended uses, which in turn allows users to specify what they are interested in, and find datasets that best match their needs. Section 6 in this chapter, the Outlook, spends some thoughts on this concept and its further development.

4 Issues in Life Cycle Inventory Databases

Creating and maintaining an LCI database presents issues and challenges in several aspects, including setup, maintenance, finances, quality assurance, and not the least integration into LCA software.

[8] https://nexus.openlca.org/

[9] https://www.lifecycleinitiative.org/applying-lca/lca-databases-map/

[10] Data Quality in Life Cycle Inventories

4.1 Setup

Setup here means the starting phase of a database. Since a database aims to provide a “safe modeling space” (see definitions in Sect. 1), the initial questions to consider are:

(i) Which datasets should be provided in the database?
(ii) In which “sequence” should they be created and provided?
(iii) Which modeling conventions should be followed by the database?

Also, of course, the following questions should be clarified at the setup phase:

Of the technical solution used
Of longer-term maintenance
Of financial and operational sustainability
Of quality assurance

The decisions taken at the setup phase determine the scope of the database, and eventually, ensure the success and long-term usability of the database. Current and previously existing databases may have taken different decisions for the setup or they have been influenced by their operators and initiators. This is evident in the varieties of LCA databases available, see Sect. 3.

Regarding the database content, i.e., the processes in the database, all databases need to solve the issue of where to start with modeling and which becomes delicate regarding closed loops existing in production systems (UNEP/SETAC 2011). For example, production of steel needs steel used in processing machinery and the production of diesel needs diesel for transport. This self-reference of LCI database systems is evidently more complicated for databases that contain aggregated processes than for databases that contain unit processes, since unit processes can be modeled also without access to, and knowledge of, the full life cycle chain. However, thinking of the consistent modeling space a database aims to provide, also a unit process database initially needs to complete supply chains with links to datasets from other databases, or already include these datasets, which in both cases raises the question of how well the other database fits to the own modeling.

Discussed here are the strategies for the setup in order to provide datasets comprehensively. For the one-sector databases (see Sect. 3), the situation is comparable, with the limitation that they never, by intention, will be able to fully provide complete life cycles.

First, a database can follow a bootstrapping approach, by starting from those processes that are most commonly used and needed by other datasets and by users. Often, these are transport and electricity, followed by construction and basic materials.

To take just one example, for “rubber sandals and slippers” from the Japanese IDEA database, the overall product system contains about 1600 individual processes, but some of them are used very often in the product system. The top five

Table 6.2 Top five most often used processes in a product system created for the Japanese IDEA database, for the product "rubber sandals and slippers" (taken from openLCA 1.8)

Processes	Number of linked inputs
331111014 electricity, Japan, 2014FY	1278
361111000 tap water	1138
181114801 energy, kerosene combustion	1094
341111801 energy, town gas 13A combustion	1092
181124801 energy, liquefied petroleum gas (LPG) combustion	1063

most used are electricity, tap water, kerosene, town gas, and liquefied petroleum gas combustion (Table 6.2).

If these datasets are initially created, they can be used many times in the product system; and if the database development focuses on those datasets that are used most often across the targeted overall datasets, the database can ideally grow, building on datasets that have already been created. This approach has been used by the Chinese CLCD database (Wang et al. 2011), where first versions contained transport and energy datasets only, with construction datasets being added in later versions.

Second, a database can start by creating datasets for several sectors and independent products in sub-projects at the same time, and share only aggregated datasets, in a limited extent, between these sub-projects. This evidently risks that datasets might become inconsistent, if several projects use differing datasets for, for example, electricity in their supply chain. Motivations for this approach might be capacity restrictions, time pressure, and the desire to involve several parties in the creation of the database early on. This approach has been used in the creation of the "EF-compliant" datasets, where about 12 different tenders have been launched to create parts of an Environmental Footprint background database.[11] Those tenders were awarded to different consultancies as well as institutes, and started with only little overlap. As a consequence, the datasets of the first of these tenders, for energy and transport, were available only for the very late data tenders, and most of the datasets could not be shared across the projects.

Third, a database can let supply chains intentionally open, in that the database creator does not attempt to provide all process datasets needed to deliver all required products, but keeps links open. Ingwersen et al. (2018) propose to rename these unfollowed products "CUTOFF," and to additionally provide "bridge processes" in the database that link then to specific background databases (Fig. 6.4).

Fourth, and final, it is possible to include datasets from other databases to complete supply chains. The license of the other database needs to permit this, and also the modeling approach should be somewhat aligned, which is often challenging. For example, the Agri-Footprint database completes agricultural dataset supply chains with aggregated datasets from ELCD (European Reference life cycle database).

[11] http://ec.europa.eu/environment/eussd/smgp/ef_pilots.htm#compliant, accessed April 21, 2019

Market for steel, unalloyed (GLO)	
Inputs	**Outputs**
Steel, unalloyed	Steel, unalloyed - GLO
Steel, unalloyed	
Transport, freight train	
Transport, freight train	
Transport, freight train	
Transport, freight train	
Transport, freight train	
Transport, freight train	
Transport, freight train	
Transport, freight train	

BRIDGEtoEBforsteelsheet	
Inputs	**Outputs**
Steel, unalloyed - GLO	CUTOFF steel sheet; light gauge; atplant

Can; light gauge steel; at plant (US)	
Inputs	**Outputs**
CUTOFF steel sheet; light gauge; at plant	Can; light gauge steel at plant - US

Fig. 6.4 Bridge processes and cutoff flows to make a database more flexible and to preempt a database from providing all products used (Ingwersen et al. 2018)

Whereas it provides its own datasets in different allocation models (price, energy, mass), the ELCD aggregated datasets cannot be changed.

Independent from the scope of the datasets and supply chains included in the database, setting up the database should also determine and set up the technical infrastructure for the database, with review workflow procedure, a tool for entering data and for moderating updates, physical databases to store the information, release channels for data, and not the least appropriate communication channels and measures.

4.2 Quality Assurance

Quality assurance is an essential part of a database, right from its creation to its long-term maintenance. A sound quality management includes the following points:

- *Goal and scope for the datasets* in a database should be clearly specified so that data quality can be determined (see Chap. 5 in this book). Ideally, the specification should cover reference time, location, the products to be modeled, and also LCA modeling issues such as system boundaries, dealing with multifunctional processes, modeling of waste, water, biogenic carbon, and long-term emissions
- *A system for assessing the quality of datasets* is in place, meaning that the data quality criteria and their assessment are specified and documented, and that a procedure and infrastructure is implemented to allow an execution of the assessment. The infrastructure includes technical tools, as well as accredited or recognized experts who can perform the review

– Conformance to the *data quality topics* mentioned in ISO 14044 is a good starting point for creating the quality guidelines for assessing the data quality standard of a database. These topics can be summarized into four key areas:
  - Representation and conformance aspects (time, geography, technology)
  - Modeling-related aspects (selected nomenclature, modeling waste, biogenic carbon, multifunctionality)
  - Measurement-related aspects (completeness, reliability of the source, uncertainty of data)
  - Procedural aspects (review procedure, copyright)

Figure 6.5 shows the review procedure followed by ecoinvent for validating a unit process. The procedure involves three different actors, including an ecoinvent manager that prepares the dataset for the database, followed by the due-diligence process carried out by two ecoinvent experts where the dataset is checked for significant issues, completeness, mathematical correctness, plausibility checks, sensitivity, uncertainty, and consistency on the basis of their quality guidelines. Corrections or modifications wherever necessary are carried out prior to the creation and documentation process. The whole process is a reiterative and takes place parallel to another until a satisfying dataset is achieved.

Datasets in a database have to undergo and pass quality assurance. If the data quality assessment includes more than a binary passed/not passed result, the assessment result, and in all cases comments regarding quality assurance of the datasets, should be provided along with the datasets.

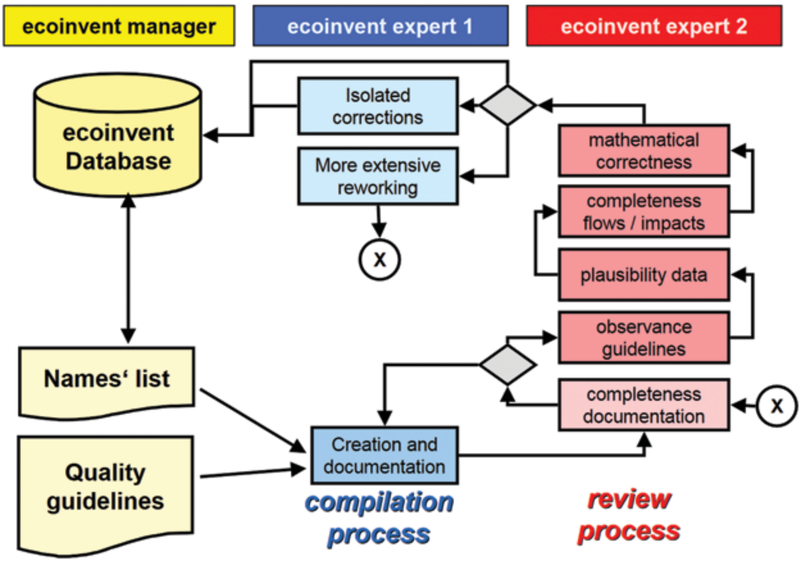

Fig. 6.5 Overview of the internal review procedure within the ecoinvent database (Frischknecht and Jungbluth 2007, p 54)

The quality of a database and of datasets in the database is crucial for the success of the database on the market. Database providers typically emphasize the performed quality assurance and review; some even provide documents about *external* quality assurance. Several frameworks exist today to address "data quality" in a database; the few notable ones are developed by:[12]

– US EPA (United States Environmental Protection Agency)
– UNEP/SETAC Life Cycle Initiative (United Nations Environment Programme, and Society of Environmental Toxicology and Chemistry)
– European Commission

For users of a database, a performed quality assurance is reassuring in that the database fulfills its purpose to provide a "safe modeling space." The detailed quality indicator results can, however, hardly be checked by a database user. For example, it is almost impossible to trace back whether a dataset refers to 2012 or 2014. This makes a clear documentation of datasets and data sources used even more important; and even more so, a documentation of the deviation from the intended goal and scope set forward for the entire database, be it intended deviation, or a deviation rather done as concession to practical requirements. This "helplessness" for a user to verify a database modeling is especially challenging for aggregated datasets where the underlying detailed model cannot be accessed by the user.

4.3 Maintenance

Maintenance of an LCI database means the provision of updates to datasets to reflect technical changes in the real world (lower emissions of cars, more efficient electricity generation, to name just two), and also the update of the database content to align with progress in LCA and especially LCIA. Newer LCIA methods often create a need for more detailed elementary flow sets (from "dust" to "PM 2.5", for example, see Chap. 9 in this book),[13] and it is typically expected that a database is expanded, i.e., contains an increasing number of datasets over time.

Maintenance is often a survival issue for databases. There is a long list of databases that disappeared after some time, despite having been created with initially enough funding and resources. It is commonly stated that database maintenance is important (UNEP/SETAC 2011), but when a database project is initiated, it is typically unclear what its long-term future looks like.[14] Funding for a continuation might typically be in sight only after a successful first project.

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[12] For US EPA, see "Data Quality", Chap. 5, Sect. 3.5.2, for UNEP/SETAC, see GLAD, Global Life Cycle Access to Data, Chap. 5, Sect. 3.5.3; for European Commission, see Environmental Footprint, Chap. 5, Sect. 3.5.1)

[13] The link between life cycle inventory analysis and life cycle impact assessment

[14] Since no database starts with guaranteed financial support over an unlimited time

While predicting the future for one given database project is difficult, it is easier to identify elements that contribute to a longer-term existence and maintenance of the database. These are:

- Financial support from public sources
- License fees
- Relevance: A sufficiently sized database or relevant dataset that is requested and not available elsewhere, which are recent
- Trust: An established name, maintained with quality assurance, documentation, and communication
- Ease of access and availability

The financial aspect is not to be underestimated. In the end, an LCI database is a product that requires considerable initial effort and long-term resources for the maintenance, and thus needs a sound business plan. In particular, a new database needs to compete with other LCA databases on the market, which also requires effort.

Public support plays a significant role among the elements for database sustainability. For one, it helps to lower license fees and to provide a database that does not meet market demand initially. On the other hand, one could argue that sustainability data are common good and therefore *should* be provided for free, with public support covering the expenses, just as street lights or other infrastructure (De Rosa et al. 2017). Public support likely makes a database more prominent ("this is the database supported by the European Commission"), but it can also make progress slower and more bureaucratic, and political changes can lead to rather abrupt changes in database development, even to discontinuation. Public support consists often of only one or very few supporters, and a change in the organizational structure can put these few sources at risk.

License fee income, on the other hand, can help to focus on market needs, and is certainly a more broadly spread and stable source of income once the database is established. Reaching this level of establishment is, however, challenging, since with initially low license fee incomes, a lot of work needs to be spent on dataset creation and on establishing the required infrastructure, and in addition, a database typically competes with other existing databases on the market.

Financial aspects aside, it is always in the interest of a database to be used. Maintenance is performed also to keep and extend the user base of a database, and to keep the database relevant. Adding and updating datasets is one core aspect of maintenance. Typically, databases follow a dedicated workflow for adding and updating datasets, with several actors involved: dataset developers, reviewers, the database managing team, and users. Figure 6.6 shows a possible workflow. Dataset developers create a dataset, send it to a reviewer, who checks the dataset following a database-wide data quality approach, writes a report, sends it (probably condensed to review criteria results) back to the developer, or to the database manager, who checks and validates it in terms of whether the dataset represents what it is intended to represent. There might be iteration loops between this validation, the review process and review criteria assessment. If the dataset is found sufficient, it is integrated into the database, possibly first in a staging version of the database. Otherwise, the

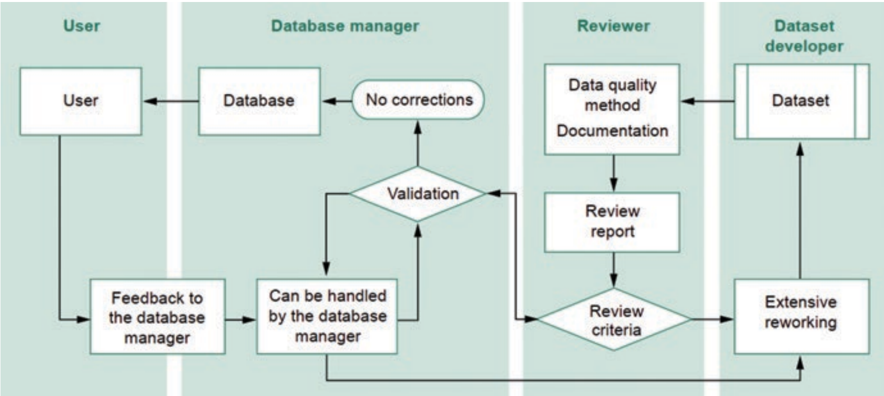

Fig. 6.6 Overview of a database management structure with focus on dataset creation and update (UNEP/SETAC 2011, p. 94)

dataset is improved by the database management team or by the dataset developer. Finally, database users provide feedback to the database management team, which is hopefully considered.

A database can be extended and updated with new large projects, in a more organic way using license fees. It can also be updated by third parties that provide and contribute to the datasets, thereby using the database as a publication platform and benefit from the review procedure including quality assurance of the database.

4.4 Integration into LCA Software

Technical accessibility of a database typically helps increasing the user base. In the end, a database will not be used primarily stand-alone, but to calculate and understand life-cycle impacts, which requires calculation software. It is therefore in the interest of a database to collaborate with software providers, and to ease the integration of the database into LCA software. Therefore, all major databases are now partnering with LCA software providers, either to establish contractual relationships that enable software companies to resell the databases, withholding a reseller rebate and thus creating an incentive for the software provider, or to provide the database in one of the common LCA data exchange formats to allow easy import of the database by the software users directly.

Only very few databases are created, supported, and provided by an LCA software developing company.[15] On the other hand, only very few databases are published without being either integrated in the software or available in an exchange

[15] For example, Thinkstep, with the GaBi LCA software and the various GaBi databases, and GreenDelta, with the PSILCA social LCA database.

format; one exception was the FEFCO database of the European Paper and Cardboard association that was provided on a printed brochure only until about 2015.

While the integration of databases in LCA software is often essential to reach users, it requires adapting the database to the structure of the software in two main ways:

1. Information contained in the database needs to be mapped to the available fields in the LCA software database and user interface. Information that is not considered in the software can either be put in comment fields or omitted. Two examples are provided:

   - The ecoinvent database considers exchange properties that describe water and carbon content and other properties, of every exchange. For example, for an emission of a tin ion, the carbon and water content are reported. These properties are not included in any LCA software so far.
   - The datasets tendered by the European Commission for the Environmental Footprint changed the way to model locations in 2018. Previously, one flow had one location assigned (emission of ammonia to air in the Netherlands). Now, a so-called exchange, i.e., a flow that is input or output of a process, has the location assigned (emission of ammonia to air in the Netherlands, from animal husbandry); this avoids the creation of thousands of flows for all different locations, but requires that the impact assessment calculation considers the exchanges instead of the flows, which is not supported so far by any of the major LCA software packages, and it requires of course that the software can store and show in the user interface the location of the exchanges.

2. The database flow nomenclature needs to be adapted often to fit the nomenclature and categories of the software. There, several different compatibility situations can occur: an exact match (=), less generic to more generic (<), more generic to less generic (>), and proxy (~).

Figure 6.7 illustrates cases for database integration in an LCA software. Suppose a database is to be mapped to the software, with its internal database structure and software-specific LCA reference data. The black circular icons represent elements that are present in the respective structures. The question mark across the element of either the database or the software indicates that the particular element is missing in one of them. Where there are elements matching between the database and the software, the match could be in either four ways. Considering example flows (or reference flows) of citrus fruits, match 1, "=," is a full match, for example, when the flow is citrus fruits in both databases. Match 2 and 3 ("<" and ">") indicate more generic mappings, where the more generic flow (e.g., fruit) is in case 2 on the software side and in case 3 on the database side. Case 4, finally, is a proxy mapping, "~"; in the example, a citrus flow might be mapped to a flow representing an orange. This simple example is valid for any of the information in the database, and for any information considered by the software.

A combination of different LCA databases into one software raises additional considerations. Taking one database as the attempt to provide one harmonized,

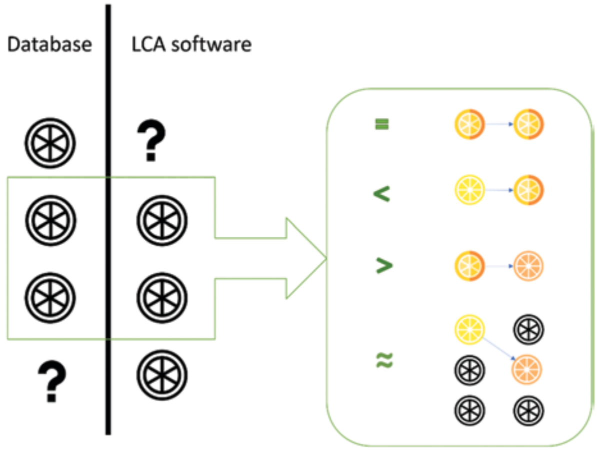

Fig. 6.7 Database integration in an LCA software, mapping cases. For further explanation, see Sect. 4.4

consistent modeling space calls for a user- or software-provided strategy to deal with data from different model perspectives and concepts in one software.

5 Data Exchange

5.1 Information in LCI to Be Exchanged

As shown in Fig. 6.1, all the information in an LCA allows data exchange.

For a process dataset, which is often exchanged, Fig. 6.8 presents further details, as proposed by ISO/TS 14048 (ISO/TS 14048: 2002), and adds administrative information, such as dataset owner, dataset creation date, among others, as well as documentation of modeling and quality assurance. Box 5.2.3 in the figure represents the exchange data that primarily contains the input and output flows, their respective direction, amount, and flow property, and is further supported by data quality information, including parameters or dataset-specific formulae, among others. Further, administrative and modeling information can be provided for flows, for product systems, and LCIA methods, for example.

5.2 Exchange Formats

Some sort of exchange formats for LCA data existed as early as around 1980 when the first LCI and LCA databases appeared. The release of the ISO/TS 14048 standard attempted to align the different concepts, by proposing a data documentation

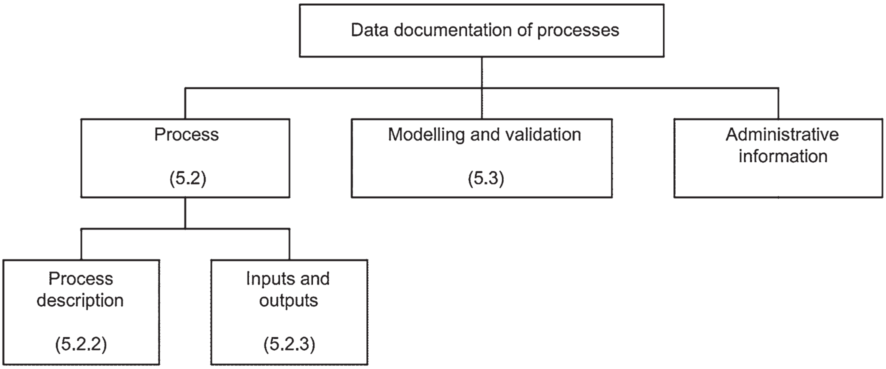

Fig. 6.8 Data documentation elements for a process dataset, as proposed by ISO/TS 14048

format for processes as shown in Fig. 6.6. Since then, all newly released formats for LCA data refer to ISO 14048/TS and can be considered compliant.

A software-integrated database differs technically on the basis of its linking concepts, size, documentation fields, field separators, to name a few, and is probably not directly accessible without the LCA software. Most databases have to be further modified and adapted to different LCA software. Typically, a database is designed for a specific software; however, it is not user-friendly to switch software for including different databases. An exchange format promises to contain "the important" information and allow an exchange from one user to another, and even from one software to another, without considering the software-internal database structure.

Over time, also the exchange formats for LCA have evolved. Nowadays, four formats are frequently used, see the following. Three of the four formats are XML formats, i.e., they follow the extensible markup language.[16] One format follows JSON-LD, Java Script Object Notation for Linked Data.[17]

EcoSpold 1[18] is the format initially released with the ecoinvent2 database, created for the ecoinvent center. It is the oldest of the ISO 14048 compliant exchange formats that is still in use. The file format goes back to an association created in the 1990s by a group of companies and researchers, forming the Society for the

[16] XML was first proposed by the W3C consortium in 1998 with the idea to provide a language that is usable over the internet, easy to write and to process, with formal and concise design, among other things (https://www.w3.org/TR/1998/REC-xml-19980210). It has been broadly adopted since.

[17] JSON-LD was developed with support from search engines, to overcome some disadvantages of XML in data interchange; it is now a recommendation of W3C (https://www.w3.org/TR/json-ld/). In JSON, data is not organized in a hierarchical tree as in XML but in a "map" (https://www.educba.com/json-vs-xml/), with simple annotations, with makes processing faster and the overall format less heavy. JSON-LD is simply speaking JSON for linked data, so that the format can directly represent ontologies for example.

[18] https://www.ecoinvent.org/files/ecospold1_data_exchange_format.zip

Promotion of Life-Cycle Data (SPOLD) with the aim to create one common format for LCA. This initiative led to the creation of the first SPOLD data format.[19] It is relatively easy, cannot distinguish processes from products, and does not understand parameters. The format is supported by almost all existing LCA software systems. Result is typically one single XML file for one process.

EcoSpold02[20] is the format developed on behalf of the ecoinvent center for the ecoinvent 3 database. This format understands parameters, unique identifiers, and distinguishes processes, flows, units, and other elements. It furthermore has many different, detailed features, for example, properties for exchanges. Being also an XML format, it has so far only been implemented in the openLCA software, apart from ecoinvent's own dataset editing software ecoEditor that is not intended for LCA calculation.

ILCD[21] is the format developed for the Joint Research Center (JRC) as reaction of some shortcomings of the EcoSpold1 format. It was released before EcoSpold02, and the first supporting database was ELCD. Being an XML-based format, it understands unique identifiers, parameters, and distinguishes processes, flows, unit groups, and other elements. All these elements are provided in one folder structure, as single XML files, and overall as one zip archive. Several extension formats exist meanwhile, for example, the ILCD+EPD format to specifically address environmental product declarations.

JSON-LD,[22] finally, is the newest of the formats, developed in JSON-LD, for openLCA. It supports parameters and unique identifiers. Similar to the ILCD format, it distinguishes different elements for an LCA model (product system processes, flows, etc.), which are stored in a folder structure and can be exchanged as a zip archive. Due to the more efficient information storage, datasets need roughly 50% of the space of the ILCD format; the datasets link directly to semantic web and ontology spaces.

Overall, data formats are quite different in the way they store information (file format) and also in details, but they all cover the majority of information to be exchanged. However, not all formats have mandatory fields to be considered by other formats.

One important aspect is that the exchange format is not necessarily identical to the format in which a database stores information. Rather, it is literally meant for *exchanging* information. Databases can thus be designed to support several data formats.

[19] Weidema B. SPOLD '99 format – an electronic data format for exchange of LCI data (1999.06.24) https://lca-net.com/files/sis.pdf

[20] https://www.ecoinvent.org/files/documentation_on_ecospold2_format.v1.0.13.zip

[21] https://eplca.jrc.ec.europa.eu/LCDN/developerILCDDataFormat.xhtml

[22] http://greendelta.github.io/olca-schema/

5.3 Interoperability Concepts

Formats with differing ways to present information, and LCA users relying not only on one single, coherent modeling space but on different approaches (e.g., due to regional conventions and innovations), created the need to address interoperability in LCA data and databases. Consequently, several elements have been developed to meet this demand; they comprise:

- A format converter to convert between different LCA exchange formats.[23] An alternative approach is to use the import and export features of LCA software. This was done in the GLAD server where the openLCA software with its import and export interfaces is integrated to enable data format conversion.[24]
- A better alignment of data formats, to prevent clashes between data formats, where mandatory fields in one data format have no corresponding field in another one.
- Mapping files to align categories and nomenclature for flows and other elements.[25]
- A deeper understanding and possible conversion of modeling-related aspects, which is, to some extent, the aim of the GLAD system (see Chap. 5, this book[26]).

It seems fair to say that these elements, despite being useful, at present do not fully permit a fluent switch from one database to another, or a seamless combination of different databases. One reason is certainly that a seamless combination of different databases somewhat contradicts the original idea of a database as one harmonized modeling space; increasing diversity in databases and increasing user demand might, in future, indeed allow this combination and enable this shift.

6 Outlook

Databases constitute a foundation for today's large, comprehensive LCA case studies, and yet, creation and maintenance require considerable effort, and exchange across different databases is not fully solved today. We expect that smarter ways for collecting data become increasingly important to make data collection faster, less error-prone, and easier. It can also be expected that data exchange, also across different software systems and different modeling choices, becomes standard, and that eventually the data material collected in databases will gain in more comprehensiveness and topicality, with possibly event-based information to be added. Novel IT developments can play a role. The JSON-LD format might replace today's prevalent

23 https://github.com/GreenDelta/olca-converter

24 https://github.com/GreenDelta/olca-conversion-service

25 https://github.com/USEPA/Federal-LCA-Commons-Elementary-Flow-List/tree/master/fedelemflowlist

26 Data quality in life cycle inventories

XML for data exchange formats, and blockchain approaches might be used for documenting supply chain interactions, see, for example, Kim and Laskowski (2018). Still, providing and maintaining an interoperable, relevant database will probably always be challenging, and there is probably no easy “silver bullet” technical solution. It seems hard to believe that one single technology, be it blockchain or other, will be able to provide a perfect solution; rather, a balanced portfolio of new and established technologies as well as procedures seem to have the potential to indeed change the way databases for life cycle inventories will be used in future, hopefully leading to more reliable, comprehensive, interoperable, and relevant LCI databases.

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Chapter 7
Algorithms of Life Cycle Inventory Analysis

Michael Srocka and Flavio Montiel

Abstract Algorithms are an essential part of a life cycle assessment (LCA) study. In this chapter, algorithms for calculating and analyzing life cycle inventory (LCI) results are described. These algorithms transform the inventory data of a product system into the information on which the impact assessment is based. It is shown how product systems can be translated into computable structures and how the latter are used to algorithmically compute the inventory results. It is also demonstrated how this formalism allows linking the product system to background databases containing thousands of unit process datasets. In this way, sources of impacts can be tracked down deeply in the supply chain paths.

Keywords Algorithms · Elementary flows · Final demand vector · Intervention matrix · Inventory results · Life cycle assessment (LCA) · Life cycle inventory analysis (LCI) · LCI calculations · LCI databases · Leontief inverse · Matrix-based LCI algorithms · Product systems · Reference product · Scaling vector · Sequential approach · Technology matrix · Unit processes

1 Introduction

Algorithms of life cycle inventory (LCI) analysis specify how to compute inventory results of product systems. A *product system* is a "collection of unit processes with elementary and product flows, performing one or more defined functions, and which models the life cycle of a product" (ISO 14040:2006). As a product system produces one functional unit, a specific amount of each elementary flow entering or leaving the product system is consumed or released. The collection of these amounts of inputs and outputs is the LCI result.

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LCI calculations are commonly performed according to matrix-based LCI algorithms. This approach to LCI calculations – there exists an established nomenclature – enabled the development of LCI databases and software that can calculate LCI results of product systems with thousands of unit processes (see Frischknecht and Kolm 1995).

This chapter describes first these standard methods for calculating LCI results in terms of linear algebra. Then it shows how to deal with some special situations such as multifunctional processes. After having described some advanced LCI analysis functions, the chapter presents some performance considerations.

Much of the formalism for LCI analysis which is presented here can be found in the original reference Heijungs (1994). This source adapted very similar methods used in input-output analysis to LCI. A more detailed reference containing many of the equations shown in this chapter, see Heijungs and Suh (2002).

2 Calculating Inventory Results

2.1 Representation with Linear Equations

This section details how product systems can be modeled in terms of linear algebra. To set the stage, some relevant terminology is fixed, which draws on to the definitions in ISO 14040:2006. A *process* consists of a set of inputs, a set of outputs, and an activity transforming the former into the latter. *Inputs* and *outputs* usually considered in LCA include "any goods or service, material or energy flow," land or the use of any of these. A *unit process* is a process for which amounts of the inputs and corresponding amounts of the outputs are specified, and that is the smallest, least aggregated process level in an inventory analysis.[1] Inputs to or outputs from a product system are *elementary flows*. All other inputs or outputs of the processes in a product system are *products.*[2]

Throughout this and the next section, apart from explicit examples, a product system is considered to be composed of $n \in N$ processes. Suppose that for each elementary flow or product featuring in this product system, a unit is specified in which it is measured everywhere. Moreover, assume that for every one of the processes we have a unit process, labeled by an integer $j \in \{1, \ldots, n\}$, quantifying some amounts of inputs and outputs to the process. These amounts need not coincide with the quantities with which the process contributes to the product system.

[1] Differentiating between processes and unit processes like this is inspired by ISO 14040:2006. Often, however, practitioners do not distinguish unit processes from processes.

[2] In contrast to ISO 14040:2006, elementary flows as introduced here can experience human transformation outside the product system. This ensures that the formalism described in this chapter is indifferent to a "system boundary". (When using LCI software, it is common to auto-complete process systems within an LCI database. This implicitly sets a system boundary.) Also, our notion of products is broader than that in ISO 14040:2006.

The first step in an LCI analysis is to shape the product system into a computable form. For this, it is assumed that unit processes are linearly scalable. This means that scaling the amounts of all inputs and outputs of a chosen unit process j by a common factor $s_j \in R$ yields another unit process.[3] Furthermore, it is assumed that the processes in the product system are (linearly) independent.[4] Thus, in assembling the product system, the amount of inputs and outputs of each unit process j can be scaled by a factor s_j specific to the unit process j.

For example, assume a product system in which a unit process emits 2 kg of CO_2 while producing 1 kg of an output product. Moreover, let there be another unit process in the product system which requires 2 kg of the output product of the first process. Then the first unit process can be scaled by a factor of 2 to fulfill this demand – while emitting 4 kg of CO_2.

Let $a_{i,j} \in R$ denote the amount (in the specified unit) of a product i in the unit process j. By convention, the amount $a_{i,j}$ is positive if i is an output and negative if it is an input of j. Abiding by this rule, the amount f_i of product i that is produced by the product system as a whole can be calculated as Eq. 7.1:

$$f_i := a_{i,1}s_1 + a_{i,2}s_2 + \ldots + a_{i,n}s_n = \sum_{j=1}^{n} a_{i,j}s_j \tag{7.1}$$

The collection over all products i featuring in the product system of the product amounts f_i that are finally delivered is the functional unit, also called the *final demand* (Heijungs and Suh 2002).

Recall that a product system models the whole life cycle of some product. Therefore, for a material product, the net output of this product is zero. Still, the use of the product can be left as an output of a homonymous process which consumed the product and maybe also outputs waste. This shows that there is always some product i for which $f_i \neq 0$. Note that we have only allowed that all inputs and outputs of a unit process be scaled by the same factor. Therefore, upon scaling the amounts of its product flows as in Eq. 7.1, also the amounts of its elementary flows are to be scaled with the same factors. Let $b_{k,j} \in R$ denote the amount (measured in the specified unit) of an elementary flow k in the unit process j (with signs as for $a_{i,j}$, i.e. $b_{k,j} > 0$ if k is an output, $b_{k,j} < 0$ if k is an input). The amount g_k of the elementary flow k that is consumed or produced by the system as a whole can be calculated as in Eq. 7.2:

$$g_k := b_{k,1}s_1 + b_{k,2}s_2 + \ldots + b_{k,n}s_n = \sum_{j=1}^{n} b_{k,j}s_j \tag{7.2}$$

These amounts of elementary flows are the *inventory result* of the product system.

[3] $s_j < 0$ enables "subtracting" the inputs and outputs of one unit process from those of another one, see Sect. 3.3.

[4] Individual inputs or outputs of two different unit processes can be correlated if they depend on a common parameter.

2.2 Reformulation with Matrices

In this section, Eqs. (7.1) and (7.2) are reformulated in terms of matrices. To this end, assume that there are $m \in N$ products in the system considered. The final demand of each of them is defined by Eq. 7.1. Combining these equations leads to Eq. 7.3:

$$\mathbf{As} = \mathbf{f} \tag{7.3}$$

where the matrix $\mathbf{A} \in \mathrm{Mat}_R(m \times n)$ with entries $a_{i,j}$ is called the *technology matrix*, the vector $\mathbf{s} \in \mathrm{Mat}_R(m \times 1)$ with components s_j the *scaling vector*, and the vector $\mathbf{f} \in \mathrm{Mat}_R(m \times 1)$ with components f_j the *final demand vector*. Often, the vector $\mathbf{f}$ has just a single nonzero entry.[5] The product that is represented by this entry is the *reference product* of the system.

Assume that there are $l \in N$ elementary flows in the product system. The contribution to the inventory result of each of these flows is given by Eq. 7.2. This system of equations can conveniently be written in matrix notation as Eq. 7.4:

$$\mathbf{Bs} = \mathbf{g} \tag{7.4}$$

The matrix $\mathbf{B} \in \mathrm{Mat}_R(l \times n)$ with entries $b_{k,j}$ is called the *intervention matrix* and the vector $\mathbf{g} \in \mathrm{Mat}_R(l \times 1)$ with components g_k is the *inventory result* for the final demand $\mathbf{f}$ of the product system.

2.3 Calculating LCI Results

The task to be considered now is to determine the inventory result of the product system described by the matrices $\mathbf{A}$ and $\mathbf{B}$ for a specified final demand $\mathbf{f}$. To achieve this, the first step is to solve Eq. 7.3 for the scaling vector $\mathbf{s}$. It is a basic fact that, to achieve this, the columns of $\mathbf{A}$ must be linearly independent. As mentioned in Sect. 2.1, it is assumed that all processes are linearly independent. Assuming additionally that every process produces some product, the columns of $\mathbf{A}$ become linearly independent. A sufficient condition for Eq. 7.3 to be solvable for $\mathbf{s}$ is that the matrix $\mathbf{A}$ be invertible. In this case, see Eq. 7.5:

$$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f} \tag{7.5}$$

Often, the number of possibilities for $\mathbf{A}$ not to be invertible is mostly reduced by assuming that the following conditions are given. On the one hand, there is the demand that each product in the product system is produced by a single process.

[5] This can always be achieved by assembling various products into a single new one by adding an additional process that has these products as inputs and produces a single product.

This implies that the corresponding technology matrix is a square matrix. Indeed, by definition, all products featuring in a product system need to be produced by some process within the product system. (All inputs or outputs not produced within the product system are elementary flows.) Furthermore, it is assumed that every process outputs some product. Consequently, if each product is the output of a single process, products correspond one-to-one to processes. Indeed, it is frequently demanded that all processes in the product system be *monofunctional*. A process is monofunctional if it has a single product as an output.[6]

Consider a technology matrix which is a square matrix and describes a product system in which all processes are monofunctional. Such a matrix is *indexed symmetrically* if the output of the j^{th} process (corresponding to unit process j in Sect. 2.1) is the j^{th} product (product j). The following fictitious example, Eq. 7.6, shows such a technology matrix together with a final demand vector:

$$\mathbf{A} = \begin{bmatrix} 0.80 & -0.12 & -0.16 \\ -0.04 & 1.20 & -0.04 \\ 0.00 & -1.32 & 0.80 \end{bmatrix}, \ \mathbf{f} = \begin{bmatrix} 0.00 \\ 2.00 \\ 0.00 \end{bmatrix} \tag{7.6}$$

If a technology matrix is indexed symmetrically, there is only one kind of loop in the product system; it describes the causation of linearly dependent columns. An archetypical example thereof, see Eq. 7.25.

For the rest of this chapter, all technology matrices are symmetrically indexed unless stated otherwise.

Solving Eq. 7.3 for **s** is an instance of reflects a standard problem in scientific computing. Consequently, there is a large number of calculation methods for solving it. Which of these methods are most appropriate depends on the structure and shape of matrix **A** (Sect. 4.4). If standard math software helps to solve the problem, it typically decides automatically the routine applied (MathWorks 2019).

The scaling vector for **A** and **f,** see Eq. 7.6, can be determined to be

$$\mathbf{s} = \begin{bmatrix} 0.86 \\ 1.79 \\ 2.96 \end{bmatrix} \tag{7.7}$$

With the following intervention matrix **B**, the LCI result **g** of the example is Eq. 7.8:

$$\mathbf{B} = \begin{bmatrix} 0.08 & 7.20 & 2.80 \\ 0.08 & 6.00 & 2.40 \end{bmatrix}, \ \mathbf{g} = \begin{bmatrix} 21.27 \\ 17.94 \end{bmatrix} \tag{7.8}$$

[6]This definition and the one of "symmetrically indexed" below assume that waste treatment is considered as an output (see Sect. 3.4); however, both definitions generalize.

2.4 The Sequential Approach

This section is devoted to an alternative method for calculating the inventory result of a product system called the *sequential approach* (Ciroth et al. 2004; Ciroth 2008). In which way this can be considered as an approximative way of solving Eq. 7.5 iteratively, see advantages toward the end of this section.

The sequential approach is essentially a graph traversal algorithm (Cormen et al. 2009) for a weighted directed graph.[7] As similar graphs reappear in Sect. 4.2, this is exemplified here for a product system with a symmetrically indexed technology matrix. A graph can be constructed to encode the information contained in this matrix as follows. As vertices, the processes are taken. The vertex corresponding to the j^{th} process is labeled by the pair $(j, a_{j,j})$. The edges of the graph represent the product flows between the processes. Hence, there is an edge between the processes j_1 and j_2 if $j_1 \neq j_2$ and $a_{j_1,j_2} \neq 0$. The direction of the edges is the direction of the product flows from output to input, e.g., from j_1 to j_2 if $a_{j_1,j_1} > 0$ and $a_{j_1,j_2} < 0$.[8] The edges are labeled by the amounts of the flows, e.g., by a_{j_1,j_2}.[9] The sequential approach as specified in Algorithm 7.1 below is a traversal algorithm for this graph. The graph corresponding to the matrix **A** introduced in Eq. 7.6 is shown in Fig. 7.1.

It is now described how the sequential approach is typically implemented – as a recursive function. The latter starts by approximating the scaling factor s_r for the unit process r providing the reference flow as

$$(s_r)_1 = \frac{f_r}{a_{r,r}} \tag{7.9}$$

Scaling the unit process r by $(s_r)_1$ creates a demand $(f_i)_1 := (s_r)_1 \cdot (-a_{i,r})$ of a product i which is an input of process r. Therefore, the scaling factor of process i is approximated as $(s_i)_1 = \frac{(f_i)_1}{a_{i,i}}$. Scaling unit process i by $(s_i)_1$ creates a demand for the inputs of this unit process, etc. This procedure may calculate several

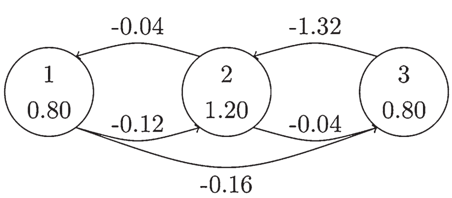

Fig. 7.1 The graph corresponding to the technology matrix in Eq. 7.6

[7] Indeed, the sequential calculation of the scaling vector **s** can be formulated as a graph search with accumulator.

[8] In the traversal algorithms corresponding to the sequential approach to calculating LCI results, the nodes are visited against this direction – as presented in Algorithm 7.1.

[9] It follows that the technology matrix is the adjacency matrix of the graph – assuming an intuitive definition of an adjacency matrix for a graph with labeled vertices and no loops at single vertices.

contributions to the scaling factor of a single unit process. This happens if there are loops or if the output of one process is used as an input by more than one other process. The respective scaling factors are to be summed,

$$s_j \coloneqq \sum_{\tau} \left(s_j\right)_{\tau} \tag{7.10}$$

This iteration is formalized in the algorithm *SEQS* in Alg. (7.1). Here, an upper limit T for the maximum number of iterations and a lower limit ϵ for the calculation accuracy are introduced. These limits are common termination conditions. Without them, the procedure does not terminate if there are loops, as, e.g., for the technology matrix in Eq. 7.6.

Algorithm 7.1 Sequential calculation of the scaling vector

function *SEQS* ($\mathbf{A}, p, f_p, \mathbf{s}, \mathbf{t}$),
    $s_p \leftarrow \dfrac{f_p}{\mathbf{A}(p,p)}$
    $\mathbf{s}(p) \leftarrow \mathbf{s}(p) + s_p$
    $\mathbf{t}(p) \leftarrow \mathbf{t}(p) + 1$
    if $\mathbf{t}(p) \geq T$ **return**
    for $q \leftarrow 1 \ldots rows(\mathbf{A})$
        if $q = p$ **continue**
        $f_q \leftarrow -\mathbf{A}(q, p) \cdot s_p$
        if $abs(f_q) > \epsilon$
            call *SEQS*($\mathbf{A}, q, f_q, \mathbf{s}, \mathbf{t}$).

Implementing the procedure *SEQS* with $\epsilon = 10^{-9}$ (and $T \geq 348$), the scaling factor in Eq. 7.7 for **A** and **f** as in Eq. 7.6 can be reproduced after iterations

$$\mathbf{t} = \begin{bmatrix} 348 \\ 306 \\ 306 \end{bmatrix} \tag{7.11}$$

The algorithm *SEQS* is in principle just a specific iterative method to solve Eq. 7.5. However, this approach lends itself to extract useful information on the product system from **A** and **f** other than the scaling vector. This includes the order in which the contributions to the scaling factors of the processes are calculated, and the number of iterations. This information can be used together with additional functions and conditions to implement, for example, the decrease of material quality in recycling loops. Also, matrix and graph-based methods can be combined to calculate advanced results like upstream contribution trees, see Section 4.2.

2.5 Relations to Input-Output Analysis

In this section, the matrix-based methods used in input-output (IO) analysis (Suh and Huppes 2005) are commented, which inspired the formulation of LCI analyses (Heijungs 1994) presented in Sect. 2.2. Furthermore, it is considered how IO analyses can interact with LCI analyses.

IO analyses (Miller and Blair 2009) involve creating (e.g., from supply and use of tables) a square coefficient matrix $\tilde{\mathbf{A}}$ whose rows and columns stand for commodities or industry sectors. (The resolution in IO statistics is characteristically much lower than in LCI data.) In fact, $\tilde{\mathbf{A}}$ is a symmetrically indexed matrix. In each column j it contains the (positive) input amounts that are required to produce one unit of product j – both measured in a fixed monetary unit. Therefore, with $\mathbf{I}$ an identity matrix of the same size as $\tilde{\mathbf{A}}$, the matrix $\mathbf{I}-\tilde{\mathbf{A}}$ is analogous to the technology matrix for a product system in which each unit process produces one unit of output.

Similarly to how LCI analyses calculate a scaling vector, an IO analysis computes a *product vector* $\mathbf{x}$ corresponding to a final demand vector $\mathbf{f}$[10] (Eq. 7.12):

$$\mathbf{x}=\left(\mathbf{I}-\tilde{\mathbf{A}}\right)^{-1}\mathbf{f} \tag{7.12}$$

Since, so far, IO analyses are completely analogous to LCI analyses, procedures, and algorithms can be transferred from the former to the latter, see, e.g., Peters (2006).

Solving Eq. 7.12 concludes classical IO analyses as they exclusively focus on economic considerations. There are, however, also environmentally extended IO (EEIO) analyses. These additionally feature a matrix $\tilde{\mathbf{B}}$ analogous to the intervention matrix $\mathbf{B}$ of LCI analyses. It is referred to as *satellite matrix*. The labels for the columns of $\tilde{\mathbf{B}}$ are the same as for $\tilde{\mathbf{A}}$ while the rows are indexed by elementary flows. Hence, the satellite matrix $\tilde{\mathbf{B}}$ can be used to compute the elementary flows involved in the activities of whole sectors of economies as

$$\tilde{\mathbf{g}}=\tilde{\mathbf{B}}\mathbf{x} \tag{7.13}$$

For EEIO analyses, there are also databases analogous to LCI databases, e.g., EXIOBASE (Wood et al. 2015) and EORA (Lenzen et al. 2012).

EEIO matrices can be merged with process-based LCI matrices for integrated hybrid analyses. This can be done, for example, by disaggregating IO matrices using process data or by completing LCI matrices with IO sector data. Furthermore, IO matrices are often linked as background data in an LCI in a tiered approach, cf. Suh and Huppes (2005):

$$\begin{bmatrix}\mathbf{s}\\ \mathbf{x}\end{bmatrix}=\begin{bmatrix}\mathbf{A} & \mathbf{Y}\\ \mathbf{X} & \mathbf{I}-\tilde{\mathbf{A}}\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{f}\\ \mathbf{0}\end{bmatrix} \tag{7.14}$$

[10] The matrix $\left(\mathbf{I}-\tilde{\mathbf{A}}\right)^{-1}$ is called the *Leontief inverse*.

In this equation, $\mathbf{A}$ is the technology matrix of a process system and $\tilde{\mathbf{A}}$ its analog in IO analysis. The matrix $\mathbf{X}$ contains the amounts of the inputs that the product system requires from the industry sectors modeled in the IO analysis. These links to the IO statistics are measured in a monetary unit. Conversely, $\mathbf{Y}$ specifies contributions of the product system to the industry sectors. In LCI analyses, however, it is particularly interesting to couple product systems to background IO databases setting $\mathbf{Y} = \mathbf{0}$.

If the EEIO analysis includes the same elementary flows as the LCI analysis, the LCI result of the hybrid system can be computed as[11]

$$\mathbf{g} = \begin{bmatrix} \mathbf{B} & \tilde{\mathbf{B}} \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \mathbf{x} \end{bmatrix} \tag{7.15}$$

3 Handling Specific Characteristics

So far, mostly, a product system has been assumed in which all processes are monofunctional and in which each product is the output of a single process. In the following sections, we consider product systems for which this is not true or which have other specific features. We show how to transform such systems in order to enable treating them as described in the preceding section.

3.1 Multiple Providers

A typical reason why Eq. 7.3 cannot be solved for $\mathbf{s}$ is that the matrix $\mathbf{A}$ is not quadratic. This problem occurs, for instance, if all processes in a product system are monofunctional but some of them output the same product. In this case, the system of equations is underdetermined. In the following example, the processes j_1 and j_2 both produce the product i_1 which is consumed by process j_3:

$$\begin{array}{cccc} & j_1 & j_2 & j_3 \\ i_1 & 1.0 & 1.0 & -1.0 \\ i_2 & 0.0 & 0.0 & 2.0 \end{array} \tag{7.16}$$

To give a common example, let the product i_1 be electricity. If the process j_3 consumes electricity from the grid, this is generically a mix of electricity produced by several distinct processes such as j_1 and j_2.

The interpretation of the equation resulting from inserting Eq. 7.16 as $\mathbf{A}$ in Eq. 7.3 in terms of LCI allows to immediately visualize why the equation is

[11] In practice, different flows may be considered in either case.

underdetermined. Namely, if Eq. 7.16 is to produce a single reference flow, this has to be the product i_2, which is not consumed by any process in the product system. In order to produce the functional unit, j_3 requires input of the product i_1. This product is produced both in process j_1 and in process j_2. These processes generically differ in which elementary flows they consume or emit. Therefore, to determine the LCI result, it is necessary to know which share of the product i_1 consumed by j_3 is produced in each of the processes j_1 and j_2, respectively. But this is not encoded in the matrix **A**. In this sense, the product system is not sufficiently determined.

The preceding considerations suggest how to achieve that Eq. 7.3 with **A** as in Eq. 7.16 becomes solvable for **s**. To wit, we may index the rows of Eq. 7.16 by pairs of processes and products. As this effectively splits the first row in Eq. 7.16, it requires that we be able to correctly distribute the input of i_1 in j_3 among the output of j_1 and j_2, e.g., as in

$$\begin{array}{cccc} & j_1 & j_2 & j_3 \\ (j_1,i_1) & 1.0 & 0.0 & -0.6 \\ (j_2,i_1) & 0.0 & 1.0 & -0.4 \\ (j_3,i_2) & 0.0 & 0.0 & 2.0 \end{array} \tag{7.17}$$

3.2 Multifunctional Processes

In this section, we consider product systems including processes which are not monofunctional. In this case, Eq. 7.3 for **s** is overdetermined. In the following example, the process j_3 produces the two products i_3 and i_4:

$$\begin{array}{cccc} & j_1 & j_2 & j_3 \\ i_1 & 1.0 & 0.0 & -0.7 \\ i_2 & 0.0 & 1.0 & -0.9 \\ i_3 & 0.0 & 0.0 & 1.8 \\ i_4 & 0.0 & 0.0 & 0.2 \end{array} \tag{7.18}$$

Similar to what we have seen in Sect. 3.1, the matrix (7.18) becomes quadratic upon labeling its columns with pairs of products and processes. This requires *allocation factors* (Heijungs and Frischknecht 1998) (real numbers contained in the interval [0, 1]) for distributing the inputs a_{i_1,j_3} of i_1 and a_{i_2,j_3} of i_2 in j_3 among the resulting columns (j_3, i_3) and (j_3, i_4). This may result in

$$\begin{array}{ccccc} & (j_1,i_1) & (j_2,i_2) & (j_3,i_3) & (j_3,i_4) \\ i_1 & 1.0 & 0.0 & -0.6 & -0.1 \\ i_2 & 0.0 & 1.0 & -0.5 & -0.4 \\ i_3 & 0.0 & 0.0 & 1.8 & 0.0 \\ i_4 & 0.0 & 0.0 & 0.0 & 0.2 \end{array} \tag{7.19}$$

The allocation factors are related to specific physical or economic properties of the products. In *causal* allocation, as in (7.19), allocation factors are specific to inputs. For *physical* or *economic* allocation, which are more typical, all inputs within one of the new columns have the same allocation factor (cf. Chap. 5 in this book).

Generally, the allocation factors applied in each row i must sum up to 1. This ensures that the total amount of the product i consumed in the processes resulting from splitting one multifunctional process j is that consumed in j.

3.3 Avoided Production

In this section, we present a second way of dealing with multifunctional processes without using allocation factors.

Assume that in the situation of (7.18) one can regard one of the coproducts of the process j_3, say i_4, as secondary. In this case, one may reason that j_3 also producing i_4 renders it unnecessary to produce i_4 in a different process j_4. In this sense, the elementary flows featuring in j_4 are avoided.

To implement the logic just presented, a unit process for j_4 is added to the technology matrix together with its upstream chain. (This means that if j_4 has inputs not provided by the processes already present in the technology matrix, collections of unit processes providing these inputs are added.) Simultaneously, the final demand for i_4 is set to zero. Starting from the matrix (7.18), this can result in the following technology matrix **A** which we depict together with a final demand vector **f** and the corresponding scaling vector **s**:

$$\mathbf{A} = \begin{bmatrix} 1.0 & 0.0 & -0.7 & -0.4 \\ 0.0 & 1.0 & -0.9 & -0.2 \\ 0.0 & 0.0 & 1.8 & 0 \\ 0.0 & 0.0 & 0.2 & 1 \end{bmatrix} \quad \mathbf{f} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad \mathbf{s} = \begin{bmatrix} 0.34 \\ 0.48 \\ 0.56 \\ -0.11 \end{bmatrix} \tag{7.20}$$

Note that the scaling factor s_4 is negative. This precisely implies that upon calculating the LCI result according to Eq. 7.4, the amounts of elementary flows featuring in j_4 are subtracted from the amounts of elementary flows featuring in the other processes.

For example, the process j_3 could model pig farming producing biogas as a secondary product. The process j_4 which is avoided could be the production of natural gas.

3.4 Waste Flows

In an LCI analysis, there are two distinct ways of dealing with waste flows. On the one hand, *waste treatment* can be treated as a product: if a process j_1 generates waste, a corresponding unit process may contain waste treatment for a quantity of waste as an input. This is provided by a process j_2 (as an output). For example, this can look like

$$\begin{array}{ccc} & j_1 & j_2 \\ i_1 & 1.0 & 0.0 \\ i_2 & -0.5 & 1.0 \end{array} \tag{7.21}$$

On the other hand, *waste* can be treated as a product. The waste resulting from the process j_1 can be considered as an output and the waste treated by the process j_2 as an input:

$$\begin{array}{ccc} & j_1 & j_2 \\ i_1 & 1.0 & 0.0 \\ i_2 & 0.5 & -1.0 \end{array} \tag{7.22}$$

Regarding the mass balance, the second method may be more appropriate. However, defining a symmetrically indexed technology matrix as in Sect. 2.3 is shorter if one considers waste treatment as a product. Also, it may be more appropriate to regard waste treatment as a reference product rather than waste. Still, both approaches are equivalent if the signs are applied consistently (including the final demand, avoided production, etc.).[12]

3.5 Loops

A product system has *loops* if processes occur in their own upstream chain. This situation is encountered frequently in LCI models. For example, a process that produces electricity may itself need electricity coming from a mix to which the process itself is one provider.

A *closed loop*, i.e., a unit process j which needs a certain amount m_j of its own product, is dealt with by subtracting the amount m_j from the output amount of the process.[13]

[12] Equation (7.1) is indifferent to an overall sign.

[13] This is exactly what happens with the amounts on the diagonal of $\mathbf{I} - \tilde{\mathbf{A}}$ in an IO analysis, cf. Sect. 2.5.

If there are at least two processes involved in a loop, it is called an *open loop*. As an example, consider a product system composed of two processes j_1 and j_2 that are linked in a loop. The corresponding technology matrix can look like

$$\begin{array}{ccc} & j_1 & j_2 \\ i_1 & 1.0 & -0.5 \\ i_2 & -1.0 & 1.0 \end{array} \tag{7.23}$$

The scaling vector resulting from (7.23) and a final demand of one unit of product j_1 is $\mathbf{s} = \begin{bmatrix} 2.0 \\ 2.0 \end{bmatrix}$.

A loop *terminates* if the scaling factors decrease over a cycle resulting in a geometric series in the sequential calculation. Continuing the example, computing the scaling factor for j_1 sequentially yields

$$s_{j_1} = 1 + 0.5 + 0.5 \cdot 0.5 + \ldots = \sum_{\tau=0}^{\infty} 0,5^{\tau} = 2.0 \tag{7.24}$$

The following loop does not terminate:

$$\begin{array}{ccc} & j_1 & j_2 \\ i_1 & 1.0 & -0.5 \\ i_2 & -1.0 & 0.5 \end{array} \tag{7.25}$$

Since the columns are linearly dependent, this cannot be solved with the matrix method. Furthermore, proceeding according to Algorithm 7.1 the scaling factors grow until the upper limit T is exceeded. This is similar for the following example, where the summands of each scaling factor double with every cycle:

$$\begin{array}{ccc} & j_1 & j_2 \\ i_1 & 1.0 & -2.0 \\ i_2 & -1.0 & 1.0 \end{array} \tag{7.26}$$

In this case, the matrix method returns the scaling vector $\mathbf{s} = \begin{bmatrix} -1.0 \\ -1.0 \end{bmatrix}$ for a demand of one unit of j_1 (the system "eats itself" – it requires more of its own output than it produces).

Loops that do not terminate need to be avoided by altering the product system. It is not possible to calculate LCI results for product systems containing such loops.

4 Advanced Analysis Functions

In this section, we present several ways of analyzing LCI results using the matrices defined in Sect. 2.3.

4.1 Direct Contributions

Assume that a product system (i.e., a technology matrix and an intervention matrix) with n processes and l elementary flows is given. Additionally, let there be a specified final demand. Then we define the *direct contribution matrix* $\mathbf{G} \in \mathrm{Mat}_R(l \times n)$ as follows. Denoting by diag($\mathbf{s}$) $\in \mathrm{Mat}_R(n \times n)$, the matrix whose only nonzero entries are $[\mathrm{diag}(\mathbf{s})]_{i,\,i} \coloneqq s_i$, we have

$$\mathbf{G} = \mathbf{B}\,diag\left(\mathbf{s}\right) \tag{7.27}$$

In the j^{th} column, the matrix **G** contains the direct contribution of the process j to the LCI result of the given product system and final demand. To illustrate a direct contribution matrix and the matrices introduced in the next section, recall the example from Sect. 2.3:

$$\mathbf{A} = \begin{bmatrix} 0.80 & -0.12 & -0.16 \\ -0.04 & 1.20 & -0.04 \\ 0.00 & -1.32 & 0.80 \end{bmatrix}, \mathbf{B} = \begin{bmatrix} 0.08 & 7.20 & 2.80 \\ 0.08 & 6.00 & 2.40 \end{bmatrix}, \mathbf{f} = \begin{bmatrix} 0.00 \\ 2.00 \\ 0.00 \end{bmatrix}, \mathbf{s} = \begin{bmatrix} 0.86 \\ 1.79 \\ 2.96 \end{bmatrix}, \mathbf{g} = \begin{bmatrix} 21.27 \\ 17.94 \end{bmatrix} \tag{7.28}$$

For these matrices, **G** looks as follows:

$$\mathbf{G} = \begin{bmatrix} 0.07 & 12.92 & 8.29 \\ 0.07 & 10.76 & 7.10 \end{bmatrix} \tag{7.29}$$

The LCI result can be obtained from **G** by summing its entries in each row[14]:

$$\mathbf{g} = \mathbf{G}\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \tag{7.30}$$

The matrix **G** can be used to perform a *dominance analysis* (Heijungs 1994). This identifies the processes that contribute dominantly to a particular elementary flow result.

Additionally, the matrix **G** can be used to filter the LCI result by specific process attributes (e.g., process locations, classifications, etc.). For this, define a vector

---

[14] Numbers in the entries of the matrices displayed are rounded – hence, they only fulfill the theoretical relations approximately.

$\mathbf{v} \equiv \mathbf{v}_{\text{attr}}$ with $v_j = 1$ if the process j has the given attribute attr and $v_j = 0$ otherwise. Then the processes having the attribute contribute the following to the result:

$$\mathbf{g}_{\text{attr}} = \mathbf{G}\mathbf{v} \tag{7.31}$$

4.2 Upstream Contributions

Let a product system with n processes, l elementary flows, and an invertible technology matrix be given. The corresponding *intensity matrix* $\mathbf{M} \in \text{Mat}_R(l \times n)$ is

$$\mathbf{M} = \mathbf{B}\mathbf{A}^{-1} \tag{7.32}$$

The matrix $\mathbf{M}$ contains in each column j the total LCI result for a final demand of one unit of the j^{th} product. Hence, if the final demand vector $\mathbf{f}$ has as single non-zero entry f_j, the LCI result is the j^{th} column of $\mathbf{M}$ times f_j. The intensity matrix of the example from Sect. 2.3, cf. (7.28), is:

$$\mathbf{M} = \begin{bmatrix} 0.63 & 10.64 & 4.16 \\ 0.55 & 8.97 & 3.56 \end{bmatrix} \tag{7.33}$$

Let a particular final demand $\mathbf{f}$ be given. Then one can extract from the intensity matrix how much each process in the product system contributes to the LCI result associated to $\mathbf{f}$. For the processes not producing the reference product, these contributions are the upstream results. To compute the latter, the total requirements $\mathbf{t} \in \text{Mat}_R(n \times 1)$ with components t_i can be employed:

$$t_i = a_{i,i} \cdot s_i \tag{7.34}$$

The total requirements of the matrices in (7.28) are as follows:

$$\mathbf{t} = \begin{bmatrix} 0.69 \\ 2.15 \\ 2.37 \end{bmatrix} \tag{7.35}$$

As long as the reference process is not part of an open loop, the upstream result of each process j is the j^{th} column of $\mathbf{M}$ multiplied by t_j.

Multiplying the second column of Eq. 7.33 by the second entry of Eq. 7.35 does, however, not result in $\mathbf{g}$ as in Eq. 7.8. Indeed, as mentioned above, the LCI result $\mathbf{g}$ is the column of $\mathbf{M}$ corresponding to the reference process times the amount of the reference flow. For the above matrices, this is the second column of (7.33) times $f_2 = 2.00$. The latter factor differs from $t_2 = 2.15$. The reason for this is as follows.

The reference product, corresponding to the second row of **A**, is an input to both the first and the third process of **A**. Hence, $t_2 = a_{2,2} \cdot s_2$ is f_2 plus the amount of product 2 consumed by the other processes. To correct for this, the following factor is introduced (r for reference):

$$c_r = \frac{s_r a_{r,r}}{f_r} \tag{7.36}$$

With the factor c_r, the upstream results $\mathbf{U} \in \mathrm{Mat}_R(l \times n)$ of all processes in the product system can be calculated for a given final demand as, cf. (7.1) for the notation:

$$\mathbf{U} = \mathbf{M} \, diag\left(c_r^{-1} \cdot \mathbf{t}\right) \tag{7.37}$$

Indeed, only the fraction $c_r^{-1} = \dfrac{f_r}{s_r a_{r,r}}$ of the amount of every product which is produced in the product system contributes to the final demand. The rest is consumed by the loop involving the reference product.

The upstream matrix corresponding to the intensity matrix (7.33), the total requirements (7.35) and the technology matrix, final demand as well as the scaling vector in (7.28) is

$$\mathbf{U} = \begin{bmatrix} 0.40 & 21.27 & 9.15 \\ 0.35 & 17.94 & 7.83 \end{bmatrix} \tag{7.38}$$

Upstream results can be visualized by Sankey diagrams (e.g., Lupton and Allwood 2017). A *Sankey diagram* is a particular graph with weighted edges. Namely, the edges represent flows between nodes. The weight of an edge corresponds to the amount of the flow and is depicted as the width of the edge.

Consider an elementary flow k. We can construct a Sankey diagram showing how much of the upstream result of k of a process j_1 can be attributed to each process j_x that uses the product of process j_1. To wit, represent each process of the product system by a node. Then, the upstream result of k of j_1 can be split into a set of weighted edges from j_1 to all j_x by applying a factor

$$c = -\frac{s_{j_x} \cdot a_{j_1, j_x}}{s_{j_1} \cdot a_{j_1, j_1}} \tag{7.39}$$

Denote by $\mathbf{u}$ the k^{th} row of $\mathbf{U}$. It contains the upstream results of k of each process in the product system. The algorithm in Alg. (7.2) shows the calculation of a Sankey diagram for **u**. For visualizing large product systems, it is often useful to reduce the number of nodes and edges of such a graph by applying a cutoff.

Algorithm 7.2 Calculating a Sankey diagram

1. **function** *SANKEY* (**A**, **s**, **u**)
2. $V \leftarrow \{\}, E \leftarrow \{\}$
3. **for** $q \leftarrow 1 \ldots rows(\mathbf{A})$
4. $add(V, Node(q, \mathbf{u}(q)))$
5. **for** $p \leftarrow 1 \ldots columns(\mathbf{A})$
6. **if** $p = q \vee \mathbf{A}(q, p) = 0$ **continue**
7. $c \leftarrow -\dfrac{\mathbf{s}(p) \cdot \mathbf{A}(q,p)}{\mathbf{s}(q) \cdot \mathbf{A}(q,q)}$
8. $weight \leftarrow c \cdot \mathbf{u}(q)$
9. $add(E, Edge(q, p, weight))$
10. **return** $Graph(V, E)$

A graph calculated by the algorithm *SANKEY* looks very much like Algorithm 7.1. Computing a Sankey diagram for the product system from Sect. 2.3 with the algorithm *SANKEY* does, however, yield different weights for the edges. They depend on the elementary flow chosen to be represented and are positive.

4.3 Contribution Trees

Contribution trees are a second means to represent upstream contributions to LCI results of a product system. As compared to Sankey diagrams, they unveil more information. Consider a product system in which a process occurs at distinct places within a supply chain. A Sankey diagram for this product system aggregates the upstream paths associated to each of these instances of the process into a single node. An upstream tree, in contrast, uses sequential scaling on the result (Bourgault et al. 2012) to expand upstream paths creating multiple instances of such processes. Thereby a structural path analysis (Defourny and Thorbecke 1984) of an inventory result can be calculated.

Let there be a product system with invertible technology matrix **A**, scaling vector **s**, LCI result **g,** and intensity matrix **M**. The algorithm below calculates an upstream tree for the LCI result $\mathbf{g}_k$ of an elementary flow k. It starts by creating the root of the tree as a node associated to the process *ref* that provides the reference product. This node is assigned the LCI result $\mathbf{g}_k$. Subsequently, the algorithm recursively adds child nodes to the tree as follows. Denote the k^{th} row of the intensity matrix **M** by **m**.

Let there be a product system with invertible technology matrix $\mathbf{A}$, scaling vector $\mathbf{s}$, LCI result $\mathbf{g}$, and intensity matrix $\mathbf{M}$. The algorithm in Alg. (7.3) calculates an upstream tree for the LCI result $\mathbf{g}_k$ of an elementary flow k. Denote the k^{th} row of the intensity matrix $\mathbf{M}$ by $\mathbf{m}$. The algorithm starts by creating the root of the tree as a node associated to the process *ref* that provides the reference product. This node is assigned the LCI result $\mathbf{g}_k$. Subsequently, the algorithm recursively adds child nodes to the tree. For example, in the second step, a node is added for the first process $\mathbf{r_1} \neq ref$ whose output is an input to the reference process. This is assigned an upstream result using the $\mathbf{r_1}^{\text{th}}$ entry of $\mathbf{m}$.

Without termination criteria, the tree resulting for a product system with loops had an infinite depth. Therefore, for example, a minimal contribution $\mathbf{u}_{\min}$ or a maximum depth $depth_{\max}$ are required (Algorithm 7.3).

Algorithm 7.3 Calculating an upstream tree

function *UTREE* ($\mathbf{A}$, s_{ref}, g_k, $\mathbf{m}$)
    $root \leftarrow Node(idx \leftarrow ref, scaling \leftarrow s_{ref}, result \leftarrow g_k)$
    call *CHILDS* ($root$, $\mathbf{A}$, $\mathbf{m}$, 0)
    return *root*
function *CHILDS* ($parent$, $\mathbf{A}$, $\mathbf{m}$, $depth$)
    if $depth > depth_{max}$ **return**
    for $r \leftarrow 1 \ldots rows(\mathbf{A})$
        if $r = parent.\,idx$ **continue**
        $v \leftarrow \mathbf{A}(r, parent.\,idx) \cdot parent.\,scaling$
        if $v = 0$ **continue**
        $child \leftarrow Node(idx \leftarrow r)$
        $child.scaling \leftarrow \dfrac{-v}{\mathbf{A}(r,r)}$
        $child.\,result \leftarrow \mathbf{m}(r) \cdot \mathbf{A}(r, r) \cdot child.\,scaling$
        $add(parent.\,childs, child)$
        if $abs(child.\,result) > u_{min}$
            call *CHILDS* ($child$, $\mathbf{A}$, $\mathbf{m}$, $depth + 1$)

Figure 7.2 shows an upstream tree for the matrices in (7.28). Note that this simultaneously visualizes the recursion tree of the sequential method.

4.4 *Relations to Impact Assessment*

As we show momentarily, the matrices describing a product system in an LCI analysis can be used in the next step of an LCA, too – the impact assessment (LCIA).

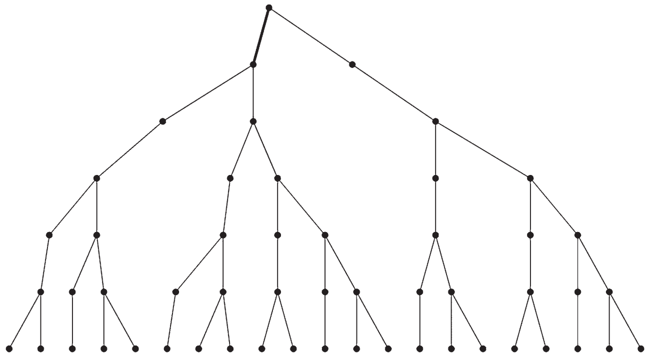

Fig. 7.2 The upstream tree of matrices in (7.28)

During an LCIA, the amounts of flows in the LCI result are aggregated into different LCIA categories using flow-specific characterization factors. From the latter we construct a matrix $\mathbf{C} \in \mathrm{Mat}_R(k \times l)$, where k is the number of LCIA categories and l the number of elementary flows. The entry $c_{y,z}$ of the matrix $\mathbf{C}$ is the characterization factor of the elementary flow z in the LCIA category$y$. The LCIA result $\mathbf{h} \in \mathrm{Mat}_R(k \times 1)$ can then be calculated as

$$\mathbf{h} = \mathbf{Cg} \tag{7.46}$$

The vector $\mathbf{h}$ contains in each row y the LCIA result of the LCIA category y. Similar to the contribution analysis described in Sects. 4.1 and 4.2, the contributions of the flows to the LCIA result can be calculated via:

$$\mathbf{H} = \mathbf{C}\,diag(\mathbf{g}) \tag{7.47}$$

Furthermore, based on the direct contributions matrix $\mathbf{G}$ and the upstream result matrix $\mathbf{U}$, the corresponding direct process contributions and upstream matrices of the LCIA results, $\mathbf{G}^* \in \mathrm{Mat}_R(k \times n)$ and $\mathbf{U}^* \in \mathrm{Mat}_R(k \times n)$, can be calculated:

$$\mathbf{G}^* = \mathbf{CG}, \mathbf{U}^* = \mathbf{CU} \tag{7.48}$$

With this, the same analysis functions as described above (dominance analysis, contribution trees, Sankey diagrams) can be calculated for the LCIA results. Also, given the matrix $\mathbf{G}$ with the LCI contributions of each process, it is possible to apply characterization factors which are specific to the regions of the respective processes (Mutel and Hellweg 2009). This enables regionalized LCIA.

5 Performance Considerations

In this section, we comment on some aspects of the technical implementation of algorithms of LCI analysis. Some of this is not yet implemented in standard LCA software. To appreciate this chapter, it is helpful to recall that LCA studies commonly employ LCI databases with thousands of unit processes consuming each other's products. Auto-completing product systems within such databases results in matrices of that size.

5.1 Selection of Algorithms

As mentioned above in Sect. 2.3, there are many algorithms to solve the equations we have presented. Here, we list some factors influencing which algorithms are most appropriate for this task. First, which algorithm performs best in calculating LCI results also depends on the hardware used. For example, computers differ in how well-suited for parallel processing they are. Further detail on this is, however, outside the scope of this chapter.

In general, when implementing the equations, matrix inversion and matrix multiplication are the most time and memory demanding operations. For square matrices of size n, they have a complexity of $O(n^{\omega})$ where $\omega > 2$ for the fastest known algorithms (Le Gall 2014). However, a full matrix inversion and matrix multiplication are only required if upstream results of all processes in the product system need to be calculated. To just evaluate the inventory result, it is enough to solve the Eqs. (7.3) and (7.4). This leaves the equation $\mathbf{f} = \mathbf{A}\mathbf{s}$ as the most demanding step.

In choosing algorithms to compute LCI results, one should consider how sparse the matrices are. To wit, process-based matrices are often very sparse. However, combining them with IO databases, cf. Section 2.5, typically results in very dense matrices. Now, there are algorithms for solving Eq. 7.3 available that massively reduce calculation time and memory usage for sparse matrices (e.g., Davis 2004; van der Vorst 1992). For dense matrices, in contrast, the amount of memory used scales comparably to the complexity.

With optimized math packages, a full matrix inversion for product systems of ten thousand of unit processes is manageable (Wang et al. 2013). Still, whether it is economic to implement this depends very much on the precise matrices considered. Indeed, in some cases, already simple iterative algorithms can outperform elaborate ones in terms of both calculation speed and accuracy (Peters 2006).

5.2 Precalculated Results

The following presents the use of distinguishing foreground and background systems in LCI analyses.

The *foreground system* of an LCI analysis comprises the processes explicitly modeled. These processes generically require inputs that are not produced within the foreground system. The processes providing these inputs are contained in the *background system* (cf. Chap. 1).

In a product system that uses an LCI database as a background system, the foreground system is typically small compared to the background system. The technology matrix of such a system is a block lower triangular matrix. Denote by $\mathbf{A_F}$ the technology matrix of the foreground system and by $\mathbf{A_B}$ that of the background system. With $\mathbf{X}$ as the inputs provided by the background system for the processes in the foreground system,

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_F} & \mathbf{0} \\ \mathbf{X} & \mathbf{A_B} \end{bmatrix} \tag{7.49}$$

The inverse of such a matrix can be calculated with the following equation (Lu and Shiou 2002)[15]:

$$\mathbf{A}^{-1} = \begin{bmatrix} \mathbf{A_F}^{-1} & \mathbf{0} \\ \mathbf{Y} & \mathbf{A_B}^{-1} \end{bmatrix} \tag{7.50}$$

where

$$\mathbf{Y} = -\mathbf{A_B}^{-1}\mathbf{X}\mathbf{A_F}^{-1} \tag{7.51}$$

For a background database, $\mathbf{A_B}^{-1}$ can be pre-calculated and stored together with the database. Moreover, $\mathbf{A_F}$ is small and $\mathbf{X}$ has only a few (sparse) columns. Therefore, the inverse $\mathbf{A}^{-1}$ of the complete technology matrix can be calculated very efficiently.

The intensity matrix of the background database, $\mathbf{M_B}$, can be precalculated, too. Then it can be combined with the intensity matrix of the foreground system $\mathbf{M_F}$:

$$\mathbf{M} = \begin{bmatrix} \mathbf{M_F} & \mathbf{M_B} \end{bmatrix} \tag{7.52}$$

$\mathbf{M_F}$ can be calculated via:

$$\mathbf{M_F} = \begin{bmatrix} \mathbf{B_F} & \mathbf{B_B} \end{bmatrix} \begin{bmatrix} \mathbf{A_F}^{-1} \\ \mathbf{Y} \end{bmatrix} \tag{7.53}$$

With this, contribution and upstream analyses can be done efficiently with pre-calculated results.

[15] It is assumed that both $\mathbf{A_F}$ and $\mathbf{A_B}$ are invertible. The latter is true if the background system is an LCI database.

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Chapter 8
Inventory Indicators in Life Cycle Assessment

Rickard Arvidsson

Abstract This chapter presents the concept of inventory indicators, which are indicators assessed at the inventory level by aggregating inventory flows at the start of the impact pathway. Although the ISO 14040 standard prescribes that a life cycle assessment (LCA) should contain an assessment of environmental impacts, inventory indicators are frequently applied for assessing energy and water use, but sometimes also for assessing waste generation, land use, material use, and emissions. For energy use, the cumulative energy demand is probably the most common indicator, which considers all renewable and non-renewable primary energy. Other energy use inventory indicators consider only non-renewable, or fossil, energy, and some consider secondary rather than primary energy. For water use, common inventory indicators include water extraction (or withdrawal), water consumption, the blue water footprint, and the green water footprint. Contrary to midpoint and endpoint indicators, inventory indicators do not consider which potential impacts the aggregated elementary flows might have. Therefore, inventory indicators have the drawback of being simplified in terms of impact modeling compared to midpoint and endpoint indicators. However, inventory indicators also have benefits: they are easy to apply, easy to interpret, and can serve as proxy indicators for damage at the endpoint level. In particular, they can be used also in cases when midpoint and endpoint characterization factors are lacking. Because of these advantages, inventory indicators are foreseen to play a role in LCA also in the future.

Keywords Abiotic resource depletion · Areas of protection · Blue water · Cumulative energy demand (CED) · Energy use · Green water · Inventory indicators · Land use · LCA · LCI · LCIA · Life cycle assessment · Life cycle impact assessment · Life cycle inventory analysis · Material use · Waste generation · Water consumption · Water footprint

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1 Introducing Inventory Indicators

In life cycle assessment (LCA), there are (at least) three levels at which environmental indicators can be constructed along the impact pathways going from emissions and resource extraction to environmental damage (Fig. 8.1). The two most frequently mentioned and used are the midpoint and endpoint levels, resulting in midpoint and endpoint indicators, respectively. Midpoint indicators are chosen at some intermediate point between the product system and the endpoint level (Hauschild and Huijbregts 2015). Examples include climate change, acidification, eutrophication, stratospheric ozone depletion, and tropospheric ozone formation. These types of indicators are the most commonly applied in LCA. The endpoint level, and consequently also endpoint indicators, correspond to the areas of protection in LCA (Hauschild and Huijbregts 2015). These are typically stated to be human health, the natural environment, and natural resources (Finnveden et al. 2009), although different names are sometimes used for these (see, e.g., Fig. 8.1). For example, the disability-adjusted life years (DALY) indicator, quantifying the years of life lost due to premature death and disability, can be applied for assessing impacts on human health at an endpoint level (Huijbregts et al. 2017). Midpoint and endpoint indicators are calculated in the characterization step of the life cycle impact assessment (LCIA) phase according to Eq. 8.1 (Hauschild and Huijbregts 2015):

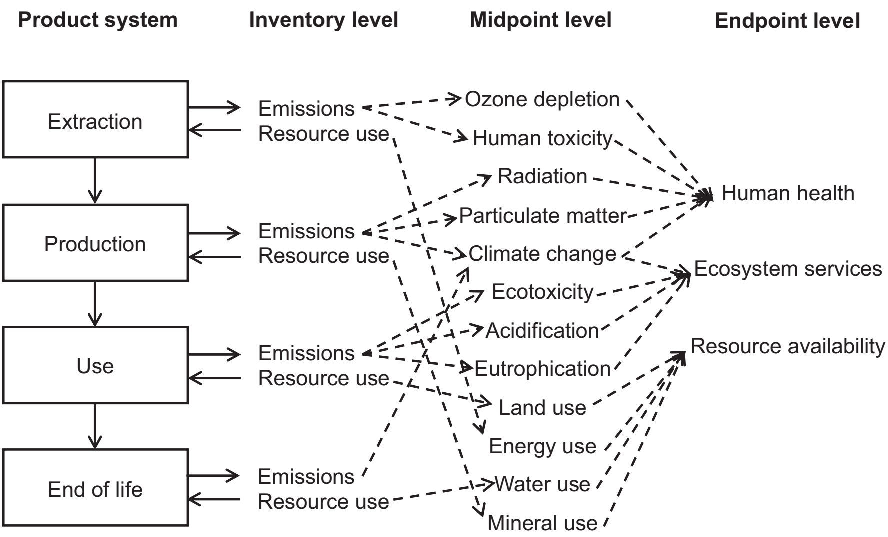

Fig. 8.1 Schematic illustration of different levels for indicator development in life cycle assessment: the inventory, midpoint, and endpoint levels. Whole arrows represent physical flows and dashed arrows represent impact pathways (Goedkoop et al. 2013, modified)

$$IS_j = \sum_i \sum_k \sum_l Q_{i,k,l} CF_{j,i,k,l} \tag{8.1}$$

where *IS* stands for impact score (e.g., climate change), CF stands for characterization factor, *Q* stands for the quantity of emission or resource extracted from the inventory, *i* is an elementary flow (emission or resource) related to the impact category *j*, *k* is the location of the emission or resource extracted, and *l* is the environmental compartment to which the emission occurs or from which the resource is extracted.

In addition to midpoint and endpoint indicators, there is another option for indicator construction in LCA: to aggregate emissions or resources already at the inventory level. In such approaches, the emission or resource quantities *Q* obtained from the life cycle inventory (LCI) analysis are summarized directly, without characterization, see Eq. 8.2:

$$I_j = \sum_i \sum_k \sum_l Q_{i,k,l} \tag{8.2}$$

where I_j is an inventory indicator related to an impact category *j*. It should be noted that according to the ISO 14040 standard, an LCA should contain an assessment of environmental impacts, which would imply that studies only using Eq. 8.2 instead of Eq. 8.1 are not actual LCA studies (ISO 2006). Despite this, as will be shown below, inventory indicators are frequently used in LCA studies (see Sects. 2, 3, and 4). Often, they are used together with midpoint indicators, but sometimes they are the only type of indicators in an LCA study. For example, a not uncommon situation in LCA studies of biofuels is to consider one inventory indicator and one midpoint indicator: energy use assessed at the inventory level (in MJ per functional unit) and climate change impact assessed at the midpoint level (in kg carbon dioxide equivalents per functional unit), see de Souza et al. (2010) for an example. Rationales and reasons for the practice of using inventory indicators are discussed in Sect. 5. An option would be to refer to studies only considering inventory indicators as "life cycle inventory (LCI) studies," a term used in the ISO 14040 standard (ISO 2006). However, since the most common practice is to use inventory indicators together with midpoint indicators, no distinction between LCI and LCA studies is made in this chapter.

The distinction between inventory and midpoint indicators is not always clear-cut. Midpoint indicators should be more closely linked to the areas of protection than are the inventory indicators, which means that midpoint indicators should reflect impacts further along the impact pathway. How much further is not specified yet. The inventory result *Q* is sometimes multiplied with a factor that, at first sight, seems akin to the characterization factor in Eq. 8.1, but at a closer look, it is questionable whether the multiplication with the factor actually takes the inventory result further along the impact pathway. For example, Frischknecht et al. (2015) used the term "characterization factor" in their paper about the cumulative energy demand (CED) indicator and stated, for example, that the characterization factor for crude oil is 45.8 MJ/kg. This use of "characterization factor" seems to imply that the CED is a midpoint indicator. However, the conversion conducted is essentially one from kg to MJ by means of the higher heating value, which is a measure of the energy content of a material. Such a conversion does not take the results notably closer to actual resource impacts (e.g., in terms of energy depletion or scarcity risk), neither would a conversion of the mass of the crude oil into volume (e.g., liters or barrels). Similarly, in the ReCiPe 2016 package of impact assessment methods, inventory-level water flows are multiplied with so-called midpoint characterization factors, specifically referred to as water requirement ratios, which reflect the extent to which water extracted is actually consumed (Huijbregts et al. 2016). For example, only 44% of the water extracted for use in agriculture is stated to be consumed, whereas the rest returns to the environment, presumably through drainage and other transport processes. Again, the use of the term "characterization factor" seems to imply that the water consumption indicator in ReCiPe 2016 is a midpoint indicator. But the water requirement ratios rather imply modifications of an elementary inventory flow (the water extracted) in order to also consider that some of the water actually flows back to the environment. It is thus rather an inventory indicator derived by subtracting one elementary flow (the water extracted) by another (the water flowing back to the environment).

In this chapter, a conservative approach is taken: in order to qualify as a midpoint indicator, factors that the inventory data is multiplied with must bring the result notably closer to midpoint impacts and not just imply some conversion of units or modification of elementary flows. The definition of an inventory indicator used throughout this chapter is thus: *an indicator that is at the same impact pathway level as the inventory data*. From this definition, it is clear that mere unit conversions and modifications of elementary flows are not sufficient to turn an inventory indicator into a midpoint indicator, since the indicator is then still at the same impact pathway level as the inventory data. Following this definition, it is maintained in this chapter that both the CED and the water consumption indicators are inventory indicators rather than midpoint indicators.

Inventory indicators are most often applied for assessing resource-related impact categories, in particular energy use and water use. Inventory indicators for these two impact categories are discussed below (Sects. 2 and 3). In Sect. 4, a number of additional inventory indicators related to waste generation, land use, material use, and emissions are discussed. In the concluding Sect. 5, the rationale behind the use of inventory indicators and their future use in LCA are discussed.

2 Energy Use Inventory Indicators

Energy use can be assessed at different levels. For example, in the ReCiPe package of impact assessment methods, fossil energy resources can be assessed at the endpoint level in terms of future cost increases due to extraction (Huijbregts et al. 2016). However, more often, energy use is assessed at an inventory level in LCA, with Q being some energy flows in Eq. 8.2. Such energy use inventory indicators are aggregated in different ways by considering different types of energy flows Q for Eq. 8.2. Arvidsson and Svanström (2016) developed a framework for energy use inventory indicators, where they outlined the following three dimensions that can be considered in such indicators:

1. The consideration of renewable energy, non-renewable energy or both.
2. The consideration of primary or secondary energy. Primary energy refers to energy resources extracted directly from nature, whereas secondary energy refers to energy commodities, such as electricity and diesel. It should be noted that since secondary energy commodities are not elementary flows, their use for indicator construction in LCA is somewhat unconventional.
3. The consideration of energy used for energy purposes only, such as for heating and electricity, or also in the form of materials not intended for energy production (sometimes called feedstock energy), such as in plastic toys and wood houses, or both.

These dimensions are important for distinguishing between the scope of different energy use inventory indicators. Whether non-renewable energy is included or not is often stated in LCA studies. Sometimes, it is also stated whether primary or secondary energy is considered. The third dimension is seldom clarified. Based on combinations of these dimensions, different energy use inventory indicators can be described.

A number of examples of energy use inventory indicators are given in Table 8.1. These energy use inventory indicators are all used in LCA practice. For example, several of them are commonly applied in LCA studies of biofuels (Arvidsson et al. 2012). Some of the energy use indicators consider energy use only, whereas others also take the energy performance of the product into account, thereby becoming more like indicators of energy efficiency. The later type of indicator is generally only applicable for assessing products that contain or generate energy, such as biofuels and solar modules. Inventory indicators of energy use and energy efficiency are described below (Sects. 2.1 and 2.2, respectively).

2.1 Inventory Indicators of Energy Use

The probably most common energy use indicator in LCA studies is the CED. It is based on the so-called energy harvested approach (Frischknecht et al. 2015). This means that the CED considers primary (i.e., not secondary) energy as extracted (i.e., harvested) from nature. Furthermore, the CED includes all kinds of energy: renewable, non-renewable, energy for energy purposes and energy for material purposes. The popularity of the CED might be linked to its early inclusion in the much-used LCA database ecoinvent (Frischknecht and Jungbluth 2004). The standard CED considers the higher heating value of materials and applies a 560,000 MJ/kg energy content for uranium. Other variants differ regarding these matters by using lower

Table 8.1 Non-exhaustive examples of energy use inventory indicators categorized according to the framework by Arvidsson and Svanström (2016)

Energy use inventory indicator	Unit	Primary (P)/ secondary (S) energy	Renewable (R)/ non-renewable (N) energy	Energy for energy (E)/ material (M) purposes	Example reference
Cumulative energy demand	MJ	P	R + N	E + M	Frischknecht et al. (2015)
Cumulative fossil energy demand	MJ	P	N	E + M	Huijbregts et al. (2006)
Secondary energy use	MJ	S	R/N/(R + N)	E/(E + M)	Davis and Sonesson (2008)
Primary renewable energy used for energy purposes (PERE)	MJ	P	R	E	EN 15804 (2013)
Primary renewable energy used for material purposes (PERM)	MJ	P	R	M	EN 15804 (2013)
Primary renewable energy total (PERT)	MJ	P	R	E + M	EN 15804 (2013)
Primary non-renewable energy used for energy purposes (PENRE)	MJ	P	N	E	EN 15804 (2013)
Primary non-renewable energy used for material purposes (PENRM)	MJ	P	N	M	EN 15804 (2013)
Primary non-renewable energy total (PENRT)	MJ	P	N	E + M	EN 15804 (2013)
Renewable secondary fuels (RSF)	MJ	S	R	E	EN 15804 (2013)
Non-renewable secondary fuels (NRSF)	MJ	S	N	E	EN 15804 (2013)
Net energy balance (or gain or value)	MJ	P/S	R/N/(R + N)	E/(E + M)	Pleanjai and Gheewala (2009)
Energy return on investment (or net energy ratio)	–	P/S	R/N/(R + N)	E/(E + M)	Arvesen and Hertwich (2015)
Energy payback time	year	P/S	R/N/(R + N)	E/(E + M)	Espinosa et al. (2012)

The symbol "+" stands for "and." The symbol "/" stands for "or" heating values and/or somewhat different energy contents for uranium, such as 451,000 MJ/kg (Frischknecht et al. 2015). The difference in CED depending on the use of higher or lower heating values is typically <10% (Frischknecht et al. 2015). A specific variant of the CED is the cumulative fossil energy demand (CFED) (Huijbregts et al. 2006). It is similar to the standard CED but considers only fossil primary energy. Effectively, this refers to crude oil, natural gas, hard coal, lignite, and sometimes also peat. The reason for only considering fossil energy, which is not uncommon in LCA, is the higher depletion risk for such stock-type energy resources than for renewable energy resources.

Other energy use inventory indicators exist or are possible to construct (Arvidsson and Svanström 2016). An example is the use of secondary energy indicators, where energy commodities going into the foreground system are summed instead of the primary energy harvested. Davis and Sonesson (2008) conducted an LCA study of two chicken meals and presented energy use results both as primary and secondary energy use. As they point out, primary energy is subject to different conversions before becoming secondary energy, so primary energy use results are always higher than – or in the case of very efficient conversion, roughly equal to – secondary energy use results. Since the origin of the secondary energy is not necessarily traced back along its product chain, whether the secondary energy comes from renewable or non-renewable sources might not be known. It is not common to see secondary energy use inventory indicators in LCA studies.

The extent to which energy used for material purposes (feedstock energy) is considered in energy use inventory indicators is often difficult to know because this dimension is the least often clarified in LCA studies. When using indicators based on primary energy, with LCI data from databases, energy for material purposes is generally included. In cases when secondary energy is reported, the use of, for example, plastic materials in the foreground system might not be considered as energy use. The choices made in relation to such aspects are therefore important to specify.

The EN 15804 standard (2013) for environmental product declaration of construction materials prescribes the use of a number of energy use inventory indicators that can easily be described using the framework by Arvidsson and Svanström (2016). The first considers the use of renewable primary energy, excluding renewable primary energy resources used as raw materials, and is called PERE. This indicator thus considers renewable primary energy, but not energy used for material purposes. The second considers the use of renewable primary energy resources used as raw materials, called PERM. It thus considers only the renewable primary energy used for material purposes. The third considers the total use of renewable energy, called PERT. The fourth, fifth, and sixth are non-renewable variants of the three before-mentioned inventory indicators, called PENRE, PENRM, and PENRT. Note that the sum of the PERT (the total renewable primary energy) and the PENRT (the total non-renewable primary energy) is equal to the CED described above. There is also a seventh inventory indicator that considers the use of renewable secondary fuels, called NRSF, and an eighth that considers the use of non-renewable secondary fuels, called NRSF. These last two indicators thus consider secondary energy used for energy purposes (i.e., as fuels) only. Because their scope is stated to be fuels only, they only consider the energy used for energy purposes and not for material purposes. Together, these eight energy use inventory indicators cover many of the combinations possible to derive from the framework by Arvidsson and Svanström (2016).

2.2 Inventory Indicators of Energy Efficiency

Sometimes, in particular, in cradle-to-gate LCA studies of energy commodities, the energy content of the produced product is subtracted from the energy use. The typical example of such a product is a biofuel. This energy use indicator can be referred to as net energy balance (NEB), net energy value or net energy gain (in the latter case assuming that the energy content of the commodity will outweigh its energy requirement) (Nguyen et al. 2007; Prueksakorn and Gheewala 2008; Pleanjai and Gheewala 2009). In addition, the energy content of by-products is generally included as a gain in the NEB. The energy use part of the NEB indicator can consider both renewable and non-renewable primary energy, in the same way as in the CED indicator, but can also be formulated in other ways. The NEB implies a cost-benefit analysis thinking: some energy is needed to produce an energy commodity (cost), but the energy commodity can then provide energy (benefit), and the indicator quantifies the "net profit." The elementary flow considered for Eq. 8.2 is thus $Q_{net} = Q_{cost} - Q_{gain}$ (or vice versa, depending on if a negative result is interpreted as a cost or gain, which differs between studies).

A similar idea lies behind the energy return on energy investment (EROI) indicator (Arvesen and Hertwich 2015), sometimes also referred to as the net energy ratio (NER) (Prueksakorn and Gheewala 2008). It is calculated according to the following principle (Eq. 8.3):

$$\text{EROI} = \frac{\text{Energy delivered}}{\text{Energy required to deliver that energy}} \tag{8.3}$$

The idea behind the EROI is thus to relate the energy obtained in the form of an energy commodity to the energy required to deliver that energy. The energy requirement is again typically assessed as the CED or some other inventory indicator of energy use. However, in the EROI, the comparison between energy "costs" and "gains" is done by division rather than by the subtraction used in the NEB indicator. The result is thus a dimensionless ratio rather than a number in MJ. The EROI also provides a cost-benefit perspective, and most of the fossil energy commodities currently produced show EROI values >1, meaning that the energy delivered is higher than the energy requirement. For example, the EROI has been estimated at 12–16 for hard coal, 5–8 for natural gas as well as 5–6 for light and heavy fuel oil (Arvesen and Hertwich 2015).

When calculating the NEB and the EROI, it is important to be cautious about calculation details in order to ensure consistent and relevant indicator results. For example, whereas the energy requirement of the EROI is often estimated as primary energy via the CED, the energy delivered is often in the form of a secondary energy commodity. This is inconsistent because primary energy is then compared to secondary energy (Arvesen and Hertwich 2015). Preferably, the energy on both sides of the subtraction (for NEB) or division (for EROI) sign should be calculated in the same way regarding whether the indicator consideres:

– Primary or secondary energy
– Renewable and/or non-renewable energy
– Energy for energy and/or material purposes

Furthermore, it is important to be consistent regarding the use of lower and higher heating values when converting masses into energy (Arvesen and Hertwich 2015).

Another energy use inventory indicator is the energy payback time (EPBT), which represents the time until a product has produced a certain amount of energy that corresponds to the energy required for producing the product. For example, a certain amount of energy is needed to produce a wind power plant, a solar panel, or a certain amount of crude oil. These three products can then all be used to deliver energy, for example, in the form of electricity. However, they can only generate electricity at a certain rate, which means it will take a certain time to “earn back” the energy requirement. The EPBT is thus calculated as Eq. 8.4 (Bhandari et al. 2015):

$$\text{EPBT} = \frac{\text{Energy required}}{\text{Energy generated per time}} \tag{8.4}$$

This indicator has the dimension time (often in years) rather than energy. It is, however, highly energy-related and can largely be seen as the ratio between two different energy flows, where one has the unit energy per time (the denominator in Eq. 8.4) and the other has the unit energy (the nominator in Eq. 8.4). To provide an idea of the magnitude of EPBTs for some energy generation technologies, conventional solar photovoltaic technologies have EBPTs ranging from about a year to about 5 years (Espinosa et al. 2012; Bhandari et al. 2015), whereas the EPBT for wind power is a few months (Espinosa et al. 2012). For hydropower and geothermal energy, the EBPT is approximately half a year, whereas biomass combustion has a comparatively high EBPT of 5–10 years (Espinosa et al. 2012). As indicated by the availability of EBPTs for different energy production technologies, it is a popular indicator for assessing their energy efficiency. Again, however, it is important to specify the nominator and denominator of Eq. 8.4 regarding the three dimensions in the energy use inventory indicator framework by Arvidsson and Svanström (2016).

3 Water Use Inventory Indicators

Water use can be assessed at midpoint and endpoint levels. At the midpoint level, the use of water can be multiplied by a water scarcity index (WSI) that reflects local geographical water scarcity on a scale from 0 to 1 (Pfister et al. 2009). The WSI corresponds to the characterization factor in Eq. 8.1. An alternative is the Available Water Remaining (AWARE) midpoint approach developed by Boulay et al. (2018), where inventory-level water use is multiplied by a characterization factor ranging from 0.1 to 100. The characterization factors from the AWARE method represent the available water remaining per area once the demands of humans and aquatic ecosystems have been met. At the endpoint level, impacts on human health from disease and malnutrition resulting from water scarcity can be estimated in terms of DALY (Boulay et al. 2011). More common, however, is to assess water use based on inventory indicators. Table 8.2 provides a non-exhaustive list of water use inventory indicators. These can be divided into two groups: classical inventory-level water use indicators in LCA and the water footprint family, although one of the water footprint members much resembles the classical water use inventory indicators.

3.1 Water Extraction and Consumption

The most classical type of water use inventory indicator is probably the water depletion indicator in the ReCiPe 2008 package of impact assessment methods (Goedkoop et al. 2013), where "depletion" refers to extraction. It simply adds water extracted from lakes, rivers, the ground (i.e., groundwater), and from unspecified natural origin, following Eq. 8.2 with the extracted water flows corresponding to Q. In a newer version of ReCiPe from 2016, factors called water requirement ratios have been added to reflect the extent to which water extracted is actually consumed

Table 8.2 Non-exhaustive examples of water use inventory indicators

Water use inventory indicator	Unit	Scope	Example reference
Water extraction or withdrawal	m^3	Water extracted from lakes, rivers, the ground and from unspecified natural origin	Goedkoop et al. (2013)
Water consumption	m^3	Like water extraction but considers that some water flows back to nature	Huijbregts et al. (2016)
Water turbined	m^3	Water flowing through hydropower dams	Humbert et al. (2012)
Blue water footprint	m^3	Consumptive use of freshwater and groundwater (similar to water consumption)	Hoekstra et al. (2011)
Green water footprint	m^3	Rain water that does not run off or recharge groundwater, but becomes stored in the soil or on top of the soil or vegetation	Hoekstra et al. (2011)

(Huijbregts et al. 2016). For example, only 44% of the water extracted for use in agriculture is stated to be consumed, whereas the rest returns to the same or similar environment, from which it can be extracted again. The addition of such return flows results provides a more accurate and relevant inventory modeling of water flows. It illustrates the important difference between water extracted and water consumed, where the first quantifies the “gross extraction” and the latter rather quantifies the “net extraction.” The elementary flow used in Eq. 8.2 for this water use inventory indicator is thus $Q_{\mathrm{net}} = Q_{\mathrm{extracted}} – Q_{\mathrm{returned}}$. However, in some cases, such as domestic and industrial use of groundwater, the water returning is generally negligible (Huijbregts et al. 2016), making the water extracted equal to the water consumed in that case. The IMPACT2002+ package of impact assessment methods includes two water use inventory indicators: water withdrawal (i.e., extraction) and water consumption (Humbert et al. 2012). The first is similar to the water extraction indicator in ReCiPe 2008 and the second is similar to the water consumption indicator in ReCiPe 2016. In addition, IMPACT2002+ has a separate indicator for water flowing through hydropower dams, called water turbined, which can be seen as a special case of water extraction. It is indeed possible to distinguish also between other specific flows of water extracted or consumed, such as surface waters from rivers, lakes or estuaries, as well as groundwater (Owens 2001).

3.2 The Water Footprint Family

A popular set of water use inventory indicators is provided within the scope of the water footprint (WF) (Hoekstra et al. 2011). It contains three distinct indicators. The first is called the blue water footprint (BWF), which is the consumptive use of freshwater and groundwater. Consumptive use of water is defined as using water that (i) evaporates, (ii) is incorporated into products, (iii) is not returned to the same catchment area from which it came, or (iv) is not returned within the same period (e.g., withdrawn during a drought and returned during a wet period). However, it does not include the water returned to its original source. In this sense, the BWF is similar to the water consumption indicators in ReCiPe 2016 and IMPACT2002 +.

The types of water mentioned so far, such as surface water and groundwater, are commonly included in water use inventory indicators in LCA. It is less common to include rain water as water use, because the rain would have fallen regardless of whether there is agricultural land below or not, and is therefore not considered to cause any impacts (Milà i Canals et al. 2009; Peters et al. 2010). However, the second indicator within the WF family, the green water footprint (GWF), considers rain that does not run off or recharge groundwater, but becomes stored in the soil, on top of the soil, or on top of vegetation (Hoekstra et al. 2011). It can be calculated as the amount of water that either evapotranspirates from an area or becomes incorporated into a harvested crop.

An even less conventional indicator included in the WF family is the third indicator, called the gray water footprint (GrayWF). It is defined as the amount of freshwater needed to dilute emissions from a product life cycle to levels complying with water quality standards (Hoekstra et al. 2011). It is calculated by dividing the amount of emissions (unit: mass) by the difference between the water quality standard for the emission and its natural background concentration (unit: mass per volume). This indicator does thus not represent actual water use, but rather pollution that makes the water unavailable for future use. According to Milà i Canals et al. (2009), both the blue and green water are inventory-level flows, making the BWF and the GWF inventory indicators. Because the GrayWF is somewhat similar to the critical volume impact assessment methods (Hauschild and Huijbregts 2015), and because it is not based on inventoried flows of water but rather on inventoried emissions, it is not considered an inventory indicator of water use here.

Note that it is possible to assess only the BWF, only the GWF, only the GrayWF, or some combination of these, including the complete WF according to Eq. 8.5:

$$\mathrm{WF} = \mathrm{BWF} + \mathrm{GWF} + \mathrm{GrayWF} \tag{8.5}$$

For common agricultural crops such as sugar beet, potato, corn, cassava, wheat, and soybean, the BWF and the GWF are roughly of the same order of magnitude (Gerbens-Leenes et al. 2009). However, in an LCA study of oil from the bush *Jatropha curcas*, the GWF was several orders of magnitude higher than the BWF (Hagman et al. 2013). This crop grew in a relatively rainy part of Mozambique and the plantation did not require any irrigation, nor any other major freshwater inputs. This might have caused the relatively high GWF and low BWF, respectively. Whether the BWF or the GWF is highest thus seems to vary between products and geographical locations. For energy commodities that are not cultivated and thus cover smaller land areas, such as fossil fuels and uranium, the BWF is often dominating.

4 Additional Inventory Indicators

There are a number of inventory indicators beyond those related to energy and water use, see Table 8.3 for some examples. Although probably applied less frequently in LCA studies compared to several of the energy and water use inventory indicators, some of them are discussed briefly here.

4.1 Waste Generation Inventory Indicators

Waste generated or landfilled throughout the product system is sometimes applied as an inventory indicator, for example, in the landfilling part of the EDIP 1997 and EDIP 2003 packages of impact assessment methods as they were implemented in the ecoinvent database (Hischier et al. 2010). The amount, typically in mass, of

Table 8.3 Non-exhaustive examples of non-energy and non-water use inventory indicators

Inventory indicator	Unit	Scope	Example references
Waste landfilled or generated	kg	Amount of waste generated or landfilled	Hischier et al. (2010)
Land use area	m^2	Amount of land required	Heijungs et al. (1997)
Material input per unit of service	kg	Amount of abiotic materials, biotic materials, eroded soil, water, and air	Schmidt-Bleek (1993)
Material footprint	kg	Amount of abiotic and biotic materials	Wiesen and Wirges (2017)
Cumulative raw material demand	kg	Amount of *utilized* abiotic and biotic materials	Giegrich et al. (2012)
Secondary material use	kg	Amount of secondary material inputs	Williams et al. (2002)
Aggregated emissions	kg	Amount of emissions generated	Tillman et al. (1991)

waste generated or landfilled corresponds to Q in Eq. 8.2 for this inventory indicator. Waste generation or waste landfilled can be presented as an aggregated amount of waste or as separate waste categories, such as bulk waste, hazardous waste, radioactive waste, slag, ashes, solid waste, and liquid waste. For example, Jönsson et al. (1997) presented results for ash, sector-specific waste, and hazardous waste in their LCA study of flooring materials. Another example is the EN 15804 standard (2013) for environmental product declaration of construction materials, which prescribes the reporting of masses of hazardous waste, non-hazardous waste and radioactive waste disposed along with the life cycles of construction materials.

4.2 Land Use Inventory Indicators

Land use involves a number of important environmental aspects, such as soil fertility, biodiversity, land fragmentation, erosion, accumulation of heavy metals, water filtration, and carbon sequestration (Mattsson et al. 2000; Koellner et al. 2013). A number of midpoint and endpoint indicators for assessing impacts of land use and land use change have been proposed, for example, related to biodiversity, biotic production, and soil quality (Antón et al. 2007; Milà i Canals et al. 2007). An alternative is to focus on the main quantitative aspect of land use, which is the amount of land area used. This approach was mentioned already by Heijungs et al. (1997). The amount of occupied land area then corresponds to Q in Eq. 8.2, measured as the land area surface (e.g., in square meters). As for waste generation, it is possible to assess the total land use or disaggregate the land use area into separate categories, such as arable land, grassland, and forest land (Heijungs et al. 1997).

4.3 Material Use Inventory Indicators

Abiotic or material resource depletion is a resource impact that has proven challenging to assess in LCA (Sonderegger et al. 2017). An alternative to assessing these impacts, which are difficult to define and capture adequately, is to apply an inventory indicator representing the sum of materials extracted (Lindfors et al. 1995; Heijungs et al. 1997). For such an indicator, the mass of material resources extracted corresponds to the amount of Q in Eq. 8.2. There are several inventory indicators that aggregate material use at the inventory level, such as the material input per unit of service (MIPS) (Schmidt-Bleek 1993), the material footprint (Wiesen and Wirges 2017), and the cumulative raw material demand (CRD, original German name: *Kumulierter Rohstoffaufwand*) (Giegrich et al. 2012). MIPS consider abiotic materials, biotic materials, eroded soil, water, and air (Ritthof et al. 2002). Contrary, the material footprint considers only abiotic and biotic materials, thus excluding eroded soil, water, and air (Wiesen and Wirges 2017). Similarly, the CRD also excludes water and air (Giegrich et al. 2012). Another important difference is that the CRD only considers materials that are utilized in society (Giegrich et al. 2012). This means that tailings and other extracted but unused materials are excluded, which is not the case for MIPS and the material footprint. It furthermore means that eroded soil is excluded, since it is not utilized in society.

These indicators generally consider the primary materials extracted, similar to primary energy as discussed in Sect. 2. However, it is also possible to consider secondary material use along the life cycle. An illustrative example of this is the study by Williams et al. (2002), which concluded that a 2 g microchip (32 MB DRAM) requires almost 2 kg of secondary materials throughout its life cycle. Most of this weight (96%) originated from fossil fuels and the rest from chemical inputs. In addition to the 2 kg, 32 kg of water and 0.7 kg of elemental gases (mainly nitrogen) were required. However, it should again be noted that the convention in LCA is that inventory results are presented in terms of elementary flows extracted from or emitted to nature and not as commodities. The use of secondary material commodities as Q in Eq. 8.2 must therefore, similar to the use of secondary energy, be regarded as unconventional.

It is possible to disaggregate inventory-level material use into several categories as well, such as into the different MIPS constituents: abiotic materials, biotic materials, eroded soil, water, and air (Ritthof et al. 2002). It is also possible to focus on one or a few key material resources only. An example of this can be found in a study by Arvidsson et al. (2018). They compared lithium-ion batteries to lithium-sulfur batteries. Lithium is a key material resource for both these two battery chemistries and might face future scarcity. Lithium use was therefore assessed separately on an inventory level in terms of kg lithium extracted per functional unit to investigate which of the batteries had the highest lithium requirement. The result showed that the lithium requirements of the two battery types were approximately of the same order of magnitude.

4.4 Emission Inventory Indicators

Emissions can sometimes be aggregated based on their masses. This was common in early LCA studies, see, for example, the study on packaging materials by Tillman et al. (1991). There can be particular reasons for applying emission inventory indicators today as well. One example is LCA studies of cars, for which air pollutants such as carbon dioxide, carbon monoxide, sulfur dioxide, nitrogen oxides, hydrocarbons, and particles emitted from combustion engines are commonly measured, compared, and regulated. It is possible to aggregate also life cycle inventory emissions in terms of these specific emissions without conducting a characterization. For example, nitrogen oxides would be summed on a mass basis instead of being characterized by their contribution to acidification and eutrophication. Similarly, hydrocarbon emissions would be summed on mass basis instead of being characterized by their contribution to ground-level ozone formation and climate change. The application of inventory indicators for such combustion-related air pollutants in LCA studies of cars could facilitate the interpretation of the results among relevant actors in automotive industries (Nordelöf et al. 2014). For example, life-cycle emissions of nitrogen oxides occurring elsewhere along the life cycle of a car could then be compared with the nitrogen oxide emissions generated by the combustion of fossil fuel in the use phase of the car.

5 Discussion and Outlook

Inventory indicators are arguably simplified since they omit important environmental and resource aspects. They ignore the fact that different quantities Q might have very different relative contributions to impact categories depending on the elementary flow i, on the location k from which the quantity is emitted or extracted, as well as on the environmental compartment l to which a substance is emitted. For example, the CED indicator makes no difference between 1 MJ energy in the form of solar electricity and 1 MJ energy in the form of crude oil extracted, despite the clear differences in resource availability between these energy resources. The water extraction indicator makes no difference between water extracted in the Atacama Desert (known as the world's driest place) and in Finland (known as "the land of a thousand lakes"). The land use area indicator does not differentiate between 1 m^2 land at an abandoned industrial site and 1 m^2 rainforest within a national park. A mere summing of emissions on a mass basis would make no difference between substances that are largely harmless (an example being water) and those that are very harmful (an extreme example being the botulinum toxin, of which 500 g suffice to kill all of mankind). Finally, an inventory-level indicator of aggregated material use does not differ between extracting 1 kg iron, with an average crustal content of about 50,000 ppm, and 1 kg gold, with an average crustal content of about 0.001 ppm. Relating the inventory indicators in these extreme examples more to actual impacts on areas of protection, for example, at some midpoint level, seems warranted. At the same time, characterization factors are highly uncertain for some impact categories. For example, the recommended characterization factors for organic substances derived using the USEtox toxicity impact assessment method have an estimated uncertainty of two orders of magnitude for ecotoxicity and three orders of magnitude for human toxicity (Rosenbaum et al. 2008). Midpoint- and endpoint-level impact assessment models thus also contain uncertainties. Whether the uncertainties arising from the lack of characterization are higher than the uncertainties arising from the characterization depends on the validity and reliability of the characterization method. For example, characterization factors for human toxicity and ecotoxicity from USEtox differ by more than 10 orders of magnitude between different substances, which is more than the 2–3 orders of magnitude uncertainty inherent in their calculation. This suggests that for the toxicity impact categories, the large difference in impact between substances is higher than the uncertainty in the characterization method, which means that although the characterization method is uncertain, it is more uncertain to merely add the emissions on a mass basis and thereby mask the many orders of magnitude difference in impact between them.

The simplicity of inventory indicators thus seems to be a clear drawback. Yet simplicity is also their strength, or rather underpins some of their strengths. Although it is easy to give extreme examples highlighting important aspects not considered by the inventory indicators, it is often less easy to capture these aspects in a relevant manner. There might not exist midpoint or endpoint indicators capturing certain aspects, or they might require additional unavailable data. The inventory indicators thus have the advantage of being possible to apply in (most) LCA studies because they require no advanced impact modeling and comparatively little data. Being easy to apply has, for example, been put forth as an argument in favor of using the material footprint indicator (Wiesen and Wirges 2017). Furthermore, even if relevant impact assessment methods do exist, the midpoint and endpoint results of such methods can be difficult for both non-experts and practitioners to interpret. To take an example, most people can understand what 1 kg substance emitted means, but fewer understand what 1 PAF m^3 day means, where "PAF m^3 day" is the unit of ecotoxicity in the USEtox method, with PAF standing for a potentially affected fraction (Rosenbaum et al. 2008). Similarly, for material use assessment, kg or metric tons of materials are probably easier to understand than MJ of exergy, the output of the cumulative exergy demand endpoint indicator (Bösch et al. 2006), and kg antimony equivalents, the output of the abiotic depletion midpoint indicator (van Oers and Guinée 2016). For inventory indicators, the drawback of simplicity is thus countered by the advantages of easiness to apply and understand. The advantage is particularly clear in situations where characterization factors are missing completely, for example, if some novel, largely unstudied substances are emitted. An example of such novel substances could be nanomaterials, where characterization factors currently exist only for a few relatively well-studied nanomaterials

(Salieri et al. 2018), thus not covering the wide range of existing nanomaterials by far. In such cases, using inventory indicators might be the only feasible alternative. The choice between inventory and other types of indicators should thus be conducted on a case-by-case basis. Clearly, there are cases when inventory indicators are useful, also in cases other than for assessing energy and water use. Two examples given in Sect. 4 are cases in point: using material use inventory indicators for certain materials (e.g., lithium) of specific interest in LCA studies of batteries (Sect. 4.3) and using emission inventory indicators for exhaust pipe emissions in LCA studies of cars (Sect. 4.4).

It has also been noted that some inventory indicators correlate relatively well with environmental impacts on midpoint and endpoint levels. Huijbregts et al. (2006) showed that the CFED indicator correlated well with several midpoint indicators, such as climate change, acidification, eutrophication, ground-level ozone formation, stratospheric ozone depletion, and human toxicity. Huijbregts et al. (2010) showed that the CED indicator also correlated well with different endpoint indicators, such as the cumulative exergy demand, the EcoScarcity method and EcoIndicator99. Furthermore, Steinmann et al. (2017) showed that four inventory indicators much akin to the CFED, the BWF, the material footprint (excluding biotic materials and fossil fuels), and the land use area (including time of occupation), respectively, together were good proxies for endpoint indicators of human health and ecosystem damage. In fact, when assessing the variation between endpoint indicator results for 976 products from cradle to gate in the ecoinvent database, the four inventory indicators accounted for >90% of the variation. Consequently, simplified inventory indicators seem to have a potential use as proxies for midpoint and endpoint indicators. Note, however, that for specific products assessed, certain inventory indicators might not be decent proxies. An example is nuclear electricity, where the CED is probably not an as decent predictor of climate change impacts as it is for many other products.

There seems to be a methodological trend toward developing midpoint indicators to replace inventory indicators. This development is perhaps clearest in the case of water use with the recent development of the AWARE method. The developers of that impact assessment method describe “the need to transition” from the water extraction and consumption indicators in Table 8.2 to a midpoint indicator that considers local water demand and availability (Boulay et al. 2018). This implies an explicit strive away from inventory indicators toward a midpoint indicator. Continued efforts in this direction are foreseen, also for other impact categories than water use. However, as noted above, inventory indicators have the advantages of being easy to apply, easy to understand, and can serve as decent proxy indicators for damage to human health and the ecosystem. Considering these benefits, inventory indicators are likely to be part of LCA for the foreseeable future, although not necessarily to the same extent and for the same impact categories as today.

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Chapter 9
The Link Between Life Cycle Inventory Analysis and Life Cycle Impact Assessment

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Abstract In this chapter, the link between life cycle inventory analysis (LCI) and life cycle impact assessment (LCIA) is discussed. For the feasibility of conducting a life cycle assessment (LCA) and for making its results more robust, it is necessary that data collected in the LCI stage are suitable for the LCIA methods, and in particular for comparative studies, it is relevant to provide matching levels of detail for all compared options. Four illustrative examples are provided: (i) the differences in receiving compartment resolution for toxic emissions, (ii) differences in stressor resolution for particulate matter formation, (iii) lacking characterization factors for metal use, and (iv) lacking characterization factors for sum parameters and not fully specified emissions (such as BOD, TOC and "alkanes, unspecified"). Two important lessons to consider for maintaining a strong link between LCI and LCIA are highlighted based on these examples. First, it is suggested that it is important to have the same resolution between LCI data and LCIA methods. Scenario analysis, where different resolutions are assumed and tested, can be a strategy in cases where differences in resolutions are unavoidable. Second, ways to handle the absence of characterization factors are discussed, including the development of additional characterization factors that match the available LCI data and derivation of characterization factors from process information.

Keywords Life cycle assessment (LCA) · Life cycle impact assessment (LCA) · Life cycle inventory analysis (LCI) · Metal scarcity · Particulate matter · Toxicity · Sum parameters · Unspecified information

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1 Introduction

A life cycle inventory analysis is often described as the most time-consuming part of a life cycle assessment (LCA) study, mainly because it is linked to collecting and validating data. An underlying assumption is then that ready-made life cycle impact assessment (LCIA) methods can be used with the collected information and that the inventory data is fit for the chosen assessment method (Guinée 2015). This means that it is vital to have guidance on what data to search for and to be able to use the data in the subsequent LCIA. One vital part of this is what data could later be purposefully used in the selected LCIA methods. If the LCIA methods selected do not include impacts from a certain stressor – or if no LCIA method at all includes an impact that is potentially linked to an emission – there is no point in searching for inventory data on emissions of that stressor from an LCA perspective. However, it could be argued that data for emissions are published in environmental reports due to a potential environmental impact, even if the cause-effect chain is not completely clear, therefore, when emission or resource demand information is available it should be considered on principle. Conversely, if there is no inventory data for a certain type of emissions – such as acidifying emissions – there is no point in including LCIA methods for impacts caused by that type of emissions. There is thus a clear link between LCI and LCIA, which follows naturally from the equation used to calculate inventory data into impact scores (*IS*) (Hauschild and Huijbregts 2015):

$$IS_j = \sum_i \sum_k \sum_l Q_{i,k,l} CF_{j,i,k,l} \tag{9.1}$$

In Eq. 9.1, CF stands for characterization factor, Q for the quantity of emission or resource use, i is a certain contributor to the impact category j, k is the location of the emission or resource use, and l is the environmental compartment to which the emission occurs or from which the resource is extracted. If no CF for the contributor i exist, there is little point in gathering data on Q for that contributor. And conversely, if there exist no data on Q for a contributor, and if it is not possible to derive data based on estimates, such as from emission factors for an individual process, the existence of a CF for the contributor is of little help. Consequently, LCI and LCIA should preferably be linked to one another, and fit together like two pieces of a puzzle (Fig. 9.1).

Such mismatches between LCI and LCIA can be of vital importance in comparative LCAs. Assume that two products A and B are being compared. For A, available data on resource use and emissions is possible to match with CFs from

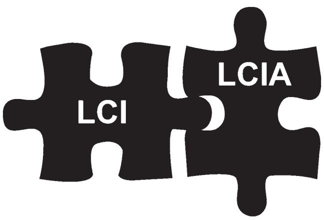

Fig. 9.1 Ideal illustration of how life cycle inventory analysis (LCI) and life cycle impact assessment (LCIA) should preferably fit together

contemporary LCIA methods. But for B, CFs might be missing for several emissions, or the resolution of the LCI data might not match that of the CFs. For example, the LCI data for B might contain many "toxic emissions to water," but as will be shown in Sect. 2, contemporary toxicity impact assessment methods need a specification regarding which type of water (fresh- or seawater). If those emissions related to B are then excluded and A receives a higher impact, it will remain unclear if B truly has lower impacts than A, or if the result is an artifact stemming from mismatches between LCI data and LCIA methods. As a short summary, for comparative studies, it is highly relevant to provide symmetry of LCI data regarding resolution and completeness.

This chapter is thus about the link between LCI and LCIA. This link is something that should be reflected upon in the goal and scope of the study, as well as iteratively throughout the whole LCA study and in particular while performing sensitivity analysis. Four illustrative examples of potential mismatches between LCI and LCIA are shown – in other words, examples when LCI and LCIA do not necessarily fit as nicely together as the illustration in Fig. 9.1 suggests. The purpose of these examples is to highlight pitfalls that can arise in an LCA study. The chapter concludes with some recommendations that will hopefully contribute to the reader being able to avoid such pitfalls in the future.

2 Receiving Compartment Resolution: The Example of Toxic Emissions

The emission of toxicants to the environment is an important problem – indeed, many historical risks that spurred regulatory responses were related to chemicals such as polychlorinated biphenyls and tributyltin (Harremoës et al. 2001). Other current chemicals risk causing severe impacts to human health and the environment include, for example, cadmium (Järup and Åkesson 2009) and endocrine disruptors (Bergman et al. 2013). Impacts from such emissions can range from local damage to ecosystem collapse and are clearly of relevance to include in LCA.

The current consensus model for assessing toxicity impacts in LCA is called USEtox, which has been developed as part of the Life Cycle Initiative of the United Nations Environment Programme and the Society for Environmental Toxicology and Chemistry (Hauschild et al. 2008; Rosenbaum et al. 2008). The currently most recent version of USEtox – version 2.01 – can be found on its webpage usetox.org, along with information and documentation about the underlying model. Still in use is also the USES-LCA 2.0 model (Huijbregts et al. 2000), which is the base for toxicity assessment used in the most recent version of the LCIA package ReCiPe from 2016 (Huijbregts et al. 2016; Huijbregts et al. 2017) and also included in the baseline set proposed by CML for midpoint indicators (Guinée et al. 2002). These two methods differ in a number of regards. For example, the measurement units for the toxicity impacts in USEtox are increased morbidity cases per kg substance for human toxicity and PAF m^3 day per kg substance for ecotoxicity, where PAF stands for potentially affected fraction of species. For USES-LCA, the measurement unit for both human toxicity and ecotoxicity is 1,4-DCB equivalents, where DCB stands for the reference substance dichlorobenzene. The USES-LCA model includes three different ecotoxicity impact categories (freshwater and marine water ecotoxicity potential as well as terrestrial ecotoxicity potential). The authors of USEtox chose to include only freshwater ecotoxicity as an impact category due to lack of experimental data for terrestrial and marine ecosystems (Rosenbaum et al. 2008).

Another notable difference is that they consider emissions to different environmental compartments. USEtox considers emissions to the eight compartments indoor air, industrial indoor air, urban air, continental rural air, continental freshwater, continental seawater, continental natural soil, and continental agricultural soil. USES-LCA considers emissions to the five compartments air, freshwater, seawater, agricultural soil, and industrial soil. By "consider," we here mean that CFs are provided for emissions to these compartments. See Fig. 9.2 for an illustration of the coverage of the two models. USEtox consequently has a higher resolution regarding the air compartment, whereas the two models have the same resolution for the water compartment. Regarding the soil compartment, they both include agricultural soil, but USEtox includes natural soil and USES-LCA includes industrial soil.

The question for LCA practitioners is whether the compartment resolutions of these two models map with available inventory data? Some data – in particular old data or data found in non-LCA databases and sources, including environmental and sustainability reports based on mandatory data required by supervisory

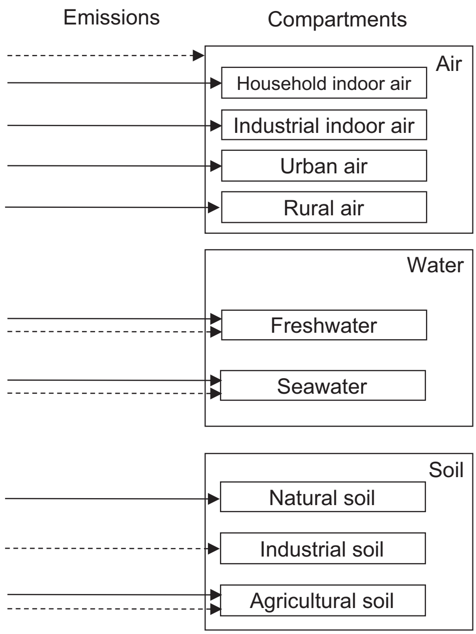

Fig. 9.2 Illustration of the coverage of the USEtox model (continuous lines) and the USES-LCA model (dashed lines) regarding emissions to different compartments

authorities – might not have specified the receiving compartment at all but only note that an emission occurs. In other cases, there might be a receiving compartment reported (or possible to deduce), but the resolution of the compartment is limited. For example, emissions from road transport can be modeled and calculated based on fuel use and emission factors, for example, in models based on the Handbook Emission Factors for Road Transport (HBEFA), developed by INFRAS (Switzerland), which are currently used in Germany, Austria, Switzerland, Norway, and Sweden and supported by the Joint Research Centre (JRC) of the European Union. Air is the natural receiving compartment for such combustion-related emissions, but as noted above, the USEtox model also requires information about whether the air is urban, rural, household indoor, or industrial indoor. Clearly, the two first are the only ones of relevance for traffic-related emissions, but the HBEFA does not specify whether emissions occur in urban or rural areas. The choice of specific receiving compartment and corresponding characterization factor might have an influence on the results, for example, by a factor of 47 as shown in Table 9.1. For an LCA study using USEtox, such unspecified emission data should therefore preferably be assigned more specific receiving compartments based on other information sources.

Also, in other cases, the practitioner may need to make a qualified assumption about the receiving compartment given some knowledge about the emission, for example, assuming that volatile substances are emitted into air. Data inventoried in the often-used LCA database Ecoinvent database (2013) are clearer regarding receiving compartment, but generally only report emissions to three aggregated compartments: air, soil, and water. Whether that air is urban, rural, or even indoor is unknown, so is whether the water is fresh- or seawater or soil is industrial or agricultural. The higher resolution of the USEtox and USES-LCA models is then of little help to the (many) users of the ecoinvent database. In general, newer LCIA methods that were developed after data were published in databases could not be considered when the data were first collected, and it is not always possible to provide more detailed information with data updates.

It is perhaps easy to think that the higher resolution a model has, the better it is. However, as discussed in Sect. 1, without LCI data to fit the LCIA model, the assessment will become hindered. Providing a higher resolution in the LCIA model can thus paradoxically result in problems for the conducting of the LCA and perhaps even result in less comprehensive LCA results. For example, if emissions to soil are available in the LCI data and a low-resolution LCIA method provides CFs for

Table 9.1 Midpoint-level human toxicity characterization factors with two significant numbers from the USEtox 2.01 model for urban and rural air, respectively, using the example of tetrachloroethylene (CAS RN: 127–18-4)

Emission compartment	Characterization factor, cancer + non-cancer [10^{-7} CTUh/kg]
Urban air	0.18
Rural air	8.5

(unspecified) soil only, there is a possibility to conduct the assessment using Eq. 9.1. However, if the LCIA method provides CFs for more specified soil compartments, such as natural or agricultural soil, then the LCI data and the LCIA model do not fit together. As mentioned above, it may in some cases be possible to make a qualified assumption about a likely compartment based on available information. In other cases, one possible way to handle such a situation of resolution mismatch could be through different what-if scenarios (Höjer et al. 2008). For example, one can assume in one scenario that all soil emissions are to natural soil, and that all soil emissions are to agricultural soil in another scenario. However, if there is a large mismatch between the LCI data and LCIA models, that would result in quite many scenarios, making the interpretation step more challenging.

3 Stressor Resolution: The Example of Particulate Matter Formation

Particulate matter (PM) is an air pollutant harmful to human health, which has been reported to cause roughly three million deaths annually (WHO 2016). The damaging PM fractions are particles with diameters below 10 µm, called PM10, since they can penetrate deep into the lungs. Furthermore, smaller particles than that, with diameters below 2.5 µm, called PM2.5 are even more damaging than larger-sized PM. In LCIA, particulate matter has sometimes been included as part of the human health impact category, as in the EDIP2003 (Hauschild and Potting 2003) and USES-LCA (Huijbregts et al. 2000) methods. More recently, it has become more common to view it as a separate impact category. The question then becomes: Which particles to consider? In particular, which particle size fraction should be considered? Less than 2.5 µm, less than 10 µm, or something else?

In the ReCiPe 2008 impact assessment method, PM10 is considered (Goedkoop et al. 2013), but in the newer version of ReCiPe from 2016, PM2.5 is considered instead (Huijbregts et al. 2016). Both the IMPACT 2002+ (Humbert et al. 2012) and IMPACT World+ (Bulle et al. 2019) impact assessment methods use PM2.5. The recent recommendation from the UNEP/SETAC life cycle initiative is also an impact assessment method based on PM2.5 as input (Frischknecht and Jolliet 2016). There thus seems to be a tendency toward preferring PM2.5 over PM10.

The question is how this focus on PM2.5 in contemporary LCIA methods match available inventory data? The ecoinvent database reports particle emission data in three size ranges: (i) <2.5 µm, thus corresponding to PM2.5, (ii) >2.5 µm and < 10 µm, thus corresponding to PM10 minus PM2.5, and (iii) >10 µm, which corresponds to particle sizes not considered harmful to human health. The inventory data corresponding to the lowest of these ranges thus match the CFs reflecting PM2.5 well. The sum of the first two match CFs reflecting PM10. The second and third ranges by themselves have no CFs available that match them.

There thus seems to be a good potential for a match between LCI data and LCIA methods for PM formation, but practitioners should be aware that particle emission data can be reported for different sizes. A careful matching of particle emission data and CFs is therefore important. In cases where they do not match, there might be ways around that. For example, it is stated in the user manual for the IMPACT 2002+ method that inventory data is often available for PM10 rather than PM2.5 (Humbert et al. 2012). To account for this, they recommend to use the relationship that the PM2.5 content of PM10 in air is approximately 0.6. The PM10-based inventory data can then be multiplied by 0.6 as a correction factor to reflect PM2.5 emissions instead. Similarly, they write that the PM2.5 share of the total particular matter (PM_{tot}) is approximately 0.33, which can be used to correct inventory data reporting the total particulate matter. These correction factors can be used in cases when the LCIA method considers PM2.5 but the inventory data is reported as PM10 or PM_{tot}.

4 Missing Characterization Factors: The Example of Metal Use

Metals are important raw materials to many life cycles. For many products, the inventory consists of a considerably long list of metal input flows. For some products, the use of metals is the perhaps highest concern of the inventory. One example of this is electric vehicles, where scarcity of metals required for the batteries, such as lithium, has been reported to be a major concern for their future use (Kushnir and Sandén 2012). Another example is the use of tellurium, gallium, ruthenium, and silver that may limit the development of solar cells (Tao et al. 2011). Yet another example is liquid-crystal displays, where the use of indium is making the screens more expensive, which has spurred the development of alternative transparent and conductive materials produced from less scarce materials (Arvidsson et al. 2016). Although not all products have metal use as the most pressing issue, most products would probably have some sort of metal input in a comprehensive inventory.

Unfortunately, there is no consensus on how to assess metal use in LCA. Klinglmair et al. (2014) conducted a review of existing LCIA models for assessing abiotic resource depletion and found that there was a lack of consensus on underlying principles, but also a lack of consensus regarding which metals should have the highest abiotic resource depletion potential. For example, for one method (the CML 2002 method), aluminum was considered two orders of magnitude less impacting than iron. For another method (the EPS 2000 method), aluminum was considered two orders of magnitude more impacting than iron. Such inconsistencies point toward a potential for further development of methods for assessing metal use. Such work will require the specification of what is actually meant by metal scarcity – for instance, in terms of timeframe (Drielsma et al. 2015).

Another observation by Klinglmair et al. (2014) was that some LCIA models included many different metals, whereas others considered only a few (Table 9.2).

Table 9.2 List of life cycle impact assessment (LCIA) models for assessing metal use

Metal	Exergy	CML 2002	EI 99	EDIP 97	EPS 2000	IMPACT 2002+	ReCiPe
Aluminum	x	x	x	x	x	x	x
Antimony		x		x	x		
Arsenic		x			x		
Barium		x			x		
Beryllium		x		x	x		
Bismuth		x			x		
Cadmium		x		x	x		
Chromium	x	x	x	x	x	x	x
Cobalt		x		x	x		x
Copper	x	x	x	x	x	x	x
Gallium		x			x		
Germanium		x			x		
Gold		x		x	x		x
Indium		x			x		
Iron	x	x	x	x	x	x	x
Potassium		x			x		
Lead	x	x	x	x	x	x	x
Lithium		x			x		
Magnesium		x					
Manganese	x	x	x	x	x	x	x
Mercury		x	x	x	x	x	
Molybdenum	x	x	x	x	x	x	x
Nickel	x	x	x	x	x	x	x
Niobium		x			x		
Palladium	x	x		x	x		x
Platinum	x	x		x	x		x
Rhenium	x	x			x		
Selenium		x		x	x		
Silicon		x					
Silver	x	x		x	x		x
Sodium		x					
Strontium		x		x	x		
Tantalum		x		x	x		
Tellurium		x		x	x		
Thallium		x		x	x		
Tin	x	x	x	x	x	x	x
Titanium		x		x	x		
Tungsten		x	x	x	x		
Vanadium		x		x	x		
Yttrium		x		x	x		
Zinc	x	x	x	x	x	x	x
Zirconium		x		x	x		
Total	**14**	**42**	**12**	**29**	**39**	**11**	**15**

Which metals they include are marked by “x.” Obtained from Klinglmair et al. (2014)

Take, for example, the six scarce metals mentioned above: lithium, tellurium, gallium, ruthenium, silver, and indium. Lithium, gallium, and indium are only included in two models (CML 2002 and EPS 2000). Tellurium is included in three models (CML 2002, EDIP 97 and EPS 2000). Silver is included in five models (Exergy, CML 2002, EDIP 97, EPS 2000, and ReCiPe). Ruthenium seems not to be included in any of the reviewed models. The CML 2002 and EPS 2000 methods are the two most inclusive methods.

This lack of coverage by some abiotic resource depletion LCIA models constitutes a challenge for linking LCI to LCIA. Assume that an assessor has an inventory list with high input amounts of a seldom-included metal. She then faces the obvious choice between (i) using one of the few LCIA models that do include the metal or (ii) leave it out from the LCIA step, only report it in terms of LCI results and maybe discuss its resource impacts qualitatively. The first alternative is problematic, since the LCIA models for abiotic resource depletion are based on different principles and it is not certain that the few models that include e.g., indium are based on the principles most suitable for the study as a whole. The second alternative is also problematic, since resource impacts from one of the main inputs then remain unassessed quantitatively. There could, however, be a third alternative in some cases. Some of the LCIA models for resource depletion provide equations that can be used by the assessor to calculate additional CFs. For example, the CML 2002 method applies the Eq. 9.2 (Guinée et al. 2002):

$$ADP_i = \frac{DR_i / R_i^2}{DR_{ref} / R_{ref}^2} \tag{9.2}$$

where DR is the extraction rate (kg/year), R is the reserve of the resource (kg), i is the resource assessed, and "ref" stands for a reference material, which is antimony in the CML 2002 model. Based on this equation, the assessor can, often without too much trouble, calculate CFs for any metal she may want to assess – for instance, ruthenium. She may even alter the equation in order to adapt to other overarching assessment principles. For example, Drielsma et al. (2015) suggested that the crustal content of a metal resource may be more relevant for long-term decisions than are reserves. The provision of such equations enables the assessor to improve the coverage of the LCIA models to match that of the LCI data.

There is a fourth alternative that may be applicable in some cases, which is again to use what-if scenarios. If there is a certain input of a scarce metal for which the CF is not known and cannot be calculated based on the LCIA model chosen, a worst-case scenario may be employed in order to investigate whether that metal input could constitute a notable share of the resource impact. In the worst-case scenario, it can be assumed that the metal's abiotic resource depletion potential is equal to the highest known for any metal in that LCIA model. If, then, the input metal becomes dominant, it is a sign that its resource impacts should be further investigated. This alternative is mainly relevant when the metal with unknown depletion potential constitutes a minor part of the total metal input. If it is the dominating input on an LCI basis, multiplication with the highest known CF will only emphasize this dominance.

5 Missing Characterization Factors: The Example of Sum Parameters

Data that have to be reported to supervisory authorities are sometimes also included in the environmental and sustainability reporting of companies, in particular over series of several years that show development over time. These data are based on sum parameters that are suitable for routine measuring such as adsorbable organic halides (AOX), chemical oxygen demand (COD), biochemical oxygen demand (BOD), total suspended solids (TSS), and total organic carbon (TOC) for waste water. For emissions to air, reported data include volatile organic compounds (VOC), among others. Sum parameters are often also used as a basis in environmental permits and can be used to evaluate the technical efficiency of treatment and remediation techniques. However, sum parameters are rarely processed in LCIA methods, even though they clearly are proxies for environmental impacts. One of the reasons is that substances with different CFs are included in a sum parameter, and without further information it is not possible to identify a specific stressor. An overview of the few instances of including sum parameters in ready-made LCIA methods is shown in Table 9.3.

COD is established in several (older) methods, often with comparably low CF values. More recent methods that include CFs for COD include Ecological Scarcity, EPS, and the North American method TRACI, for which CFs are lower than for any other flow that contributes to the respective categories.

Ecological Scarcity considers regulatory emission limits and goals for Switzerland as a basis to calculate Eco-Factors and is, therefore, able to accommodate even sum parameters for which no single stressor is identified (Frischknecht and Büsser Knöpfel 2014). The categories “water pollutants” and “non-radioactive waste” included in the Ecological Scarcity method do not refer to any specific impact, but that is not required for regulatory limits to be established. This allows for flexibility in the Ecological Scarcity method regarding the inclusion of sum parameters. No other method has been identified to account for AOX and TOC.

While sum parameters are not often considered in LCIA methods, they certainly indicate that emissions occur. The level of detail in LCIA methods requires, however, more specific information that can be related to a substance or compound. Where this information is available, considering sum parameters additionally can lead to the overestimation of impacts. However, information based on single species can also be incomplete. For example, Köhler (2006) noted that the toxicity of specified individual organic contaminants in waterborne organic emissions could not

Table 9.3 Examples of sum parameters in selected LCIA methods

Sum parameter	Method	Impact category
COD (water)	Ecoindicator 95 v2.1	Eutrophication
COD (water)	CML 2002 baseline	Eutrophication
COD (water)	IMPACT 2002+	Aquatic eutrophication
COD (water)	Ecological Scarcity 2013	Eutrophication
COD (water)	TRACI v2.1	Eutrophication
COD (water)	EPS 2015	Fish and meat production capacity, Species extinction
BOD5 (water)	TRACI v2.1	Eutrophication
BOD5 (water)	EPS 2015	Fish and meat production capacity, Species extinction
AOX (water)	Ecological Scarcity 2013	Water pollutants
VOC	ILCD 2011 Midpoint v1.10	Photochemical ozone formation
VOC	IMPACT 2002+	Respiratory organics
TOC (water/groundwater long-term)	Ecological Scarcity	Non-radioactive waste to deposit

explain the ecotoxicological impacts of the emission as observed based on toxicity tests. The effluent potentially contained additional organic substances that were not listed individually but contributed to the TOC. She therefore instead attempted to develop CFs for the whole TOC parameter by considering the general fate and effects of TOC in wastewater treatment, resulting in broad ranges due to the lack of detailed data on TOC mixtures. Despite the broad CFs ranges, applying them in a scenario fashion is an attractive alternative to merely omitting the impacts of reported TOC emissions completely. Similar attempts could be made for other sum parameters and/or other industry branches than wastewater treatment.

Creating CFs specific for sum parameters is thus one strategy to create a match between LCI data and LCIA methods. Another strategy is to disaggregate sum parameters so that they fit existing CFs for more specific stressors. This requires knowledge regarding emission sources and processes. Where sum parameters are the only information available for process emissions, a first approach could then be to identify sector-specific emissions based on which substances are used in the process or, where this is not available, based on literature sources. The sum parameter can then be disaggregated into sub-components or, if the composition is not well known, different scenarios reflecting different compositions can be tested. For example, where emissions are listed as "(mineral) oils, unspecified, to river," this will not be considered in an LCIA method, despite the fact that mineral oils contain toxic organic stressors such as polycyclic aromatic hydrocarbons (Almeda et al. 2013) and inorganic stressors including a large variety of heavy metals (Fedorov et al. 2007). Further specification of the composition of oils is recommended to make sure that emissions from sources are evaluated and considered in the assessment. Information for that is, however, unfortunately not widely published, and triangulation based on several data sources needs to be carried out. The approach helps to overcome data gaps, but is still based on estimates and assumptions.

6 Discussion and Outlook

Based on the four examples above, two important lessons for linking LCI and LCIA can be identified. The first is about the resolution in the LCI data and the LCIA model. As shown for the cases of receiving compartments for toxic emissions and particulate matter fractions, a resolution mismatch can create problems for conducting an LCA study. In some cases, the practitioner may be able to make qualified assumptions to increase the resolution of the LCI data to match the LCIA model. This could, for example, be done for PM by correcting for the content of PM2.5. If not possible, different scenarios, where, for example, it is assumed that all toxic emissions to water occur to freshwater, might provide hypothetical cornerstone results. Given LCI data with low resolution, the practitioner might need to revisit the selection of LCIA methods and instead chose one with similarly low resolution. And the other way around – if the LCI data has a higher resolution than the LCIA method, an LCIA method with higher resolution might instead be selected.

We also recommend that developers of LCIA models provide recommendation on how to handle situations with more or less aggregated LCI data, e.g., if emission data for to water is available but the model requires emission data for freshwater specifically. A general note that can be made is that since LCI data acquisition is often expensive and time-consuming, it is recommendable to develop LCIA models with available LCI data in mind.

The second lesson is the importance of available CFs, as shown for the cases of metal use and sum parameters. A problematic situation with lacking CFs for important emissions and recourses is difficult to resolve in any satisfactory way. As an advanced option, a practitioner can follow Köhler (2006) and develop new CFs that match the available LCI data. As a less advanced option, scenarios might again provide some guidance. Assigning worst-case CFs to metals lacking specific CFs might tell whether the metal has any potential to constitute a hotspot in the assessment.

The examples in this chapter clearly show that problems can arise when there is a mismatch between LCI analysis and LCIA. To facilitate the application of LCA, such mismatches should therefore preferably be avoided. The examples provided here, and the two main lessons about the importance of similar resolution and availability of CFs can hopefully help reducing such mismatches in the future.

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Glossary

Aggregated process collection of multiple unit processes and/or other aggregated processes
Allocation partitioning of flows in multifunctional processes
Area of protection the safeguard objects in life cycle assessment, often human health, ecosystem quality, and natural resources
Background system part of the product system beyond the influence of a certain actor
Characterization factor factor that translates inventory data into impact scores
Data quality characteristics of data that relate to their ability to satisfy stated requirements
Dynamic LCA type of LCA that considers the temporal resolution of input and output flows
Elementary flow flow leaving or entering the natural environment
Endpoint indicator life cycle impact assessment indicators at the endpoint level, i.e., the areas of protection
Environmentally-extended input-output analysis method for developing an inventory based on accounting data
Fitness for purpose characteristics of data that relate to their ability to satisfy stated requirements
Flow movement of energy and/or materials
Flow chart graphical illustration of the studied product system, including boxes representing processes as well as arrows representing product flows
Foreground system part of the product system that a certain actor can influence
Functional flow flow that constitutes the goal of a process, such as product outputs for production processes and waste inputs for waste treatment processes
Functional unit the quantified performance of the product system, to which all flows are scaled
Input flow that enters a process

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Inventory list of elementary flows related to a product system
Inventory indicator summed quantities of certain inventory data, such as energy or water flows
Impact score the quantitative result obtained from the life cycle impact assessment
ISO 14044 standard for life cycle assessment
Life cycle assessment (LCA) tool for assessing environmental and resource impacts of products and services from a life-cycle perspective
Life cycle impact assessment (LCIA) third phase of the life cycle assessment framework, entailing the categorization and characterization of inventory data into impact scores
Life cycle inventory analysis (LCI) second phase of the life cycle assessment framework, entailing the construction of flow charts, gathering data and conducting calculations
Life cycle inventory database system for organizing, storing, and retrieving large amounts of digital inventory datasets easily
Midpoint indicator life cycle impact assessment indicators corresponding to the midpoint level, i.e., some point between the inventory level and the areas of protection
Monofunctional process unit process yielding only one functional flow
Multifunctional process unit processes yielding more than one functional flow
Multifunctionality when multiple products emanate from one process
Output flow that exits a process
Partitioning the splitting of multifunctional flows into several monofunctional flows, which can be conducted based on physical or economic bases
Pedigree matrix approach for quantifying qualitative expert judgment of uncertainty based on a number of indicators
Process node in the societal metabolism where flows meet and can be transformed
Product flow all flows that are not elementary flows
Product system set of processes connected by flows, performing one or more defined functions and modeling the life cycle of a product
Prospective LCA type of LCA tailored for assessing emerging technologies in a future, mature state of development
Substitution crediting a product system by subtracting the impacts of an alternative product system
System boundary border between the studied product system, the natural environment and other product systems
System expansion expanding the system boundary for including additional functions
Truncation error error made when developing a process-based inventory instead of one based on environmentally extended input-output analysis
Unit process least aggregated process level in a production system

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