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# D2.2 Definition of FCH-LCA guidelines

## WP2 Reformulation of current guidelines for Life Cycle Assessment

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# EXECUTIVE SUMMARY

This document presents the Life Cycle Assessment (LCA) guidelines developed within the SH2E project for fuel cells and hydrogen (FCH) systems, as a result of Task 2.3. The objectives of the present guidelines are to provide a consistent methodology that allows a robust characterisation of FCH systems and their fair comparison. Besides updating previous LCA guidelines specific to FCH systems including results and trends identified in previous tasks of the project (Tasks 2.1 and 2.2), they aim to fill gaps such as prospective assessment and material criticality (task 3.3). The implementation of the requirements and recommendations provided in the present document in an LCA software is specifically addressed in Task 2.4. The present guidelines only address the environmental dimension, while their subsequent extension to the economic and social dimensions will be implemented in WP4 (and WP5 for Life Cycle Sustainability Assessment).

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# KEY TERMS

| Term | Definition |
|---|---|
| **Allocation** | Partitioning the inputs/outputs, considering the different functions and the relationship (preferentially physical relationship) among these (1) |
| **Biogenic carbon** | $CO_2$ uptake through photosynthesis and carbon emissions ($CO_2$, CO and $CH_4$) from transformation or degradation of biomass (e.g., due to combustion, landfilling…) (2) |
| **Biogenic carbon storage** | Sequestration of carbon dioxide ($CO_2$) by living organisms, such as trees, crops and soils. Storage starts with $CO_2$ uptake via photosynthesis and ends when it is released again into the atmosphere (2) |
| **Biomass** | Organic material from plants and animals (3), such as wood, crops, organic fraction of municipal solid waste, manure |
| **Capital goods** | Components like machinery used in production processes, buildings, office equipment, transport vehicles, and transportation infrastructure (4) |
| **Carbon capture and storage (CCS)** | Capture, transport and storage of carbon dioxide ($CO_2$) in geological formations (5,6) |
| **Carbon capture and utilization (CCU)** | Capture and use of carbon dioxide ($CO_2$) to feed processes for $CO_2$ conversion into products, such as chemicals and fuels (5,6) |
| **Characterisation** | "*Calculation of category indicator results*" (1) using characterisation factors for every relevant flow, according to the analysed impact category |
| **Characterisation factor** | "*Factor derived from a characterization model which is applied to convert an assigned life cycle inventory analysis result to the common unit of the category indicator*" (1) |
| **Classification** | "*Assignment of LCI results to the selected impact categories*" (1) |
| **Cradle-to-Gate** | Life cycle assessment including all stages from resource extraction to the factory gate |
| **Cradle-to-Grave** | Life cycle assessment including all stages from resource extraction to the use and disposal phase |
| **Data** | "*Collection of facts or organized information, usually the results of observation, experience, or experiment, or a set of premises from which conclusions may be drawn. Data may consist of numbers, words, or images*" (7) |
| **Data quality** | "*Characteristics of data that relate to their ability to satisfy stated requirements*" (1) |
| **Elementary flow** | Material or energy entering the system being studied that has been drawn from the environment without previous human transformation, or material or energy leaving the system being studied that is released into the environment without subsequent human transformation (1) |
| **Functional flow** | Flow representing a function of the system. Functional flows can be product flows being produced in the considered process or waste flows being treated in the process (8) |
| **Functional unit** | Quantitative representation of the function of the system, which serves as reference for all the flows involved in the assessed system |
| **Hydrogen as a by-product** | Hydrogen produced by a system for which hydrogen production is not the main purpose of the process (e.g., steam cracking) (9) |
| **Hydrogen as a co-product** | Hydrogen produced by a system in which hydrogen and other products are key valuable outputs |
| **Hydrogen as the main product** | Hydrogen produced by a system that has as the primary goal its production (e.g., electrolysers) |
| **Fuel cell** | System that operates based on electrochemical processes and is applied in the conversion of fuels into electricity, besides thermal energy (10) |

| | |
|---|---|
| **Grouping** | "*Sorting and possibly ranking of the impact categories*" (1) |
| **Impact category** | "*Class representing environmental issues of concern to which life cycle inventory analysis results may be assigned*" (1) |
| **Impact category indicator** | "*Quantifiable representation of an impact category*" (1) |
| **Life cycle assessment (LCA)** | Methodology to quantitatively assess the potential environmental impacts of product systems from a holistic perspective (1) |
| **Life cycle impact assessment** | Third phase of the LCA framework, which aims to evaluate the environmental impacts considered in the life cycle studied (1) |
| **Life cycle inventory (LCI)** | It is the result of the second phase of the LCA framework; it contains information regarding all input and output flows referring to the system boundary (1) |
| **Life cycle inventory database** | "*System intended to organise, store, and retrieve large amounts of digital LCI datasets easily. It consists of an organised 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*" (11) |
| **Multi-functional system/process** | System/process that originates more than one functional flow (8) |
| **Non-functional flow** | Every flow excluding the functional flows (8) |
| **Normalisation** | "*Calculating the magnitude of category indicator results relative to reference information*" (1), which is basically the division of the results for every category by a reference value obtaining a number with no measurement unit |
| **Primary data (raw data)** | Data that are collected directly related to their object of study (12); there are different ways to obtain primary data: "meter readings, purchase records, utility bills, engineering models, direct monitoring, material/product balances, stoichiometry, or other methods for obtaining data from specific processes in the value chain" (2) |
| **Secondary data** | *"Data collected by someone else earlier*" (2); e.g. average industry data, specific industry data, data from literature available (e.g., peer-reviewed papers or patents) (2) |
| **Subdivision** | Division of the unit process in different sub-processes (1) |
| **System boundaries** | Set of criteria that specify which processes are included in the product system and determine which unit processes shall be included in the LCA |
| **System expansion** | Inclusion of additional functions for products that are not the quantitative reference of the process, allowing to expand the product system (1) |
| **Unit process** | "*Smallest element considered in the life cycle inventory analysis for which input and output data are quantified*" (14) |
| **Weighting** | "*Converting and possibly aggregating indicator results across impact categories using numerical factors based on value-choices*" (1) |

# ACRONYMS

| | |
|---|---|
| AEL | Alkaline Electrolyser |
| AFC | Alkaline Fuel Cell |
| CCS | Carbon Capture and Storage |
| CCU | Carbon Capture and Utilisation |
| CRM | Critical Raw Materials |
| EoL | End-of-Life |
| FCH | Fuel Cells and Hydrogen |
| LCA | Life Cycle Assessment |
| LCIA | Life Cycle Impact Assessment |
| LOHC | Liquid Organic Hydrogen Carriers |
| MCFC | Molten Carbonate Fuel Cell |
| MRL | Manufacturing Readiness Level |
| PAFC | Phosphoric Acid Fuel Cell |
| PEMWE | Proton Exchange Membrane Electrolyser |
| PEMFC | Proton Exchange Membrane Fuel Cell |
| RA | Risk Assessment |
| SMR | Steam Methane Reforming |
| SOE | Solid Oxide Electrolyser |
| SOFC | Solid Oxide Fuel Cell |
| TRL | Technology Readiness Level |

# GENERAL INFORMATION

This document provides methodological guidance on how to perform a Life Cycle Assessment (LCA) of fuel cells and hydrogen (FCH) systems. It builds on international standards and reference documents on LCA in general (ISO 14040 (14), ISO 14044 (1), and ILCD handbook (15)), as well as on previous FCH-specific guidelines (10,16). This document embraces hydrogen production, hydrogen use and hydrogen production & use systems. It promotes a harmonised and consistent evaluation of the life-cycle environmental impacts of FCH products through robust and well-defined tailor-made methods to effectively support case-specific accounting and decision-making processes. In this sense, the present document effectively incorporates the lessons learnt in previous deliverables of the SH2E project, where an exhaustive review on LCA of FCH systems was carried out (17).

The present guidelines are addressed to any LCA practitioner addressing LCA of FCH systems (hydrogen production, hydrogen use or hydrogen production & use). The practitioner is guided on how to deal with all the methodological aspects of an LCA (functional unit, system boundaries, method and impact categories, etc.) and with specific topics relevant to FCH systems (e.g. capital goods, end-of-life, biogenic carbon emissions and carbon storage, material criticality). Moreover, advanced topics are also addressed, either relevant to emerging technologies with a potentially significant market share (i.e. prospectivity and consequentiality) or scientifically relevant in the context of LCA or ecology (e.g. verification and validation, thresholds).

## How to use this document

The document provides guidance on how to conduct an LCA of FCH systems. The provisions, recommendations and supplementary information are clearly identified in the document according to the following colour code:

In the green boxes, requirements are presented.

In the light blue boxes, recommendations are presented.

In the yellow boxes, supplementary information is reported.

The different topics in the guidelines are also evaluated in terms of their “method readiness level”, i.e. a score identifying the level of development of the addressed topic within the LCA community under the following scheme:

| Method readiness level | Meaning | Symbol |
|---|---|---|
| 5 | In LCA software and databases | ●●●●● |
| 4 | In databases, data available | ●●●●○ |
| 3 | Stable | ●●●○○ |
| 2 | Discussions | ●●○○○ |
| 1 | First ideas | ●○○○○ |

# GUIDANCE ON PERFORMING LIFE CYCLE ASSESSMENT OF FCH SYSTEMS

## 1. Introduction

**Life Cycle Assessment (LCA) is a methodology to quantitatively assess the potential environmental impacts of product systems from a holistic perspective**. LCA is defined in the ISO standards 14040 and 14044 (1,14) as "*the compilation and evaluation of the inputs, outputs and the potential environmental impacts of a product system throughout its entire life cycle"* (14).

LCA considers several typologies of environmental impacts, which helps decision-makers to avoid, or at least be aware of, **burden-shifting and trade-off** issues that may appear when implementing a new product or strategy. These issues appear when a specific product or service ameliorates one specific impact category while worsening others (18). Trade-offs can also arise in the form of burden shifting from one life-cycle stage to another (e.g., environmental burdens transferred from the use phase to the manufacturing one). The inclusion of the **whole life cycle** avoids skipping those concerns and permits a better understanding of global supply chains. Since the environmental implications of the assessed system are measured on the basis of the **function** of the system, LCA also allows practitioners to compare different product systems with the same function, which makes it very valuable for decision-makers. The function of the system is expressed through the **functional unit**, which is a quantitative representation of the main function of the system (Section 3.2).

From a practical perspective, LCA is composed of four phases (1): **goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and interpretation** (Figure 1). The four phases are interconnected and information flows in both senses between LCA phases. This is in agreement with the **iterative nature** of LCA, which involves the construction of a model that is progressively improved in terms of goal (e.g., intended application), scope (e.g., system boundaries), inventory (e.g., data quality), and impact assessment (e.g., indicators to be included). The interpretation phase is crucial in this regard, searching for the influence of methodological choices, assumptions, etc. to decide whether the model could be improved, or if modifications are needed to achieve the goal of the study. The phases of an LCA can be defined as follows (10,14,16,19):

- **Goal and scope definition:** the goal defines and explains the purpose of the study, identifying the intended application(s) and the application situation or decision context. It also involves the explanation of the limits of the study based on the intrinsic LCA methodology limitations and the specific methodological choices made in the study. The scope describes the limits of the study in terms of the analysed system, its function and functional unit, life-cycle stages covered, assumptions, methodological choices, environmental impacts investigated, and impact assessment methods chosen for their quantification.

- **Life cycle inventory analysis:** systematic compilation of information regarding mass and energy balances along the life cycle. This involves the collection of data directly linked to the assessed system (**foreground system**), but also to the economic context that surrounds the product/service and with which it interacts (**background system**).

- **Life cycle impact assessment:** the flows between economic activities (**technosphere**) and the nature (**biosphere**) are characterised by considering the potential impact of substances. Several impact indicators are available to express the potential impact of substances in a common unit (characterisation step) for each impact category (e.g., climate change). Further processing of the results may be needed if impact categories are to be compared (normalisation step) or if a single indicator wants to be proposed (weighting step).

- **Interpretation:** the LCA results, both inventory and impact results, are analysed to study contributions and potential issues (e.g., high contribution of a process whose data quality may be improved). This phase includes robustness tests, sensitivity analyses, completeness analyses, and consistency checks. Data quality and uncertainty analyses can also be performed.

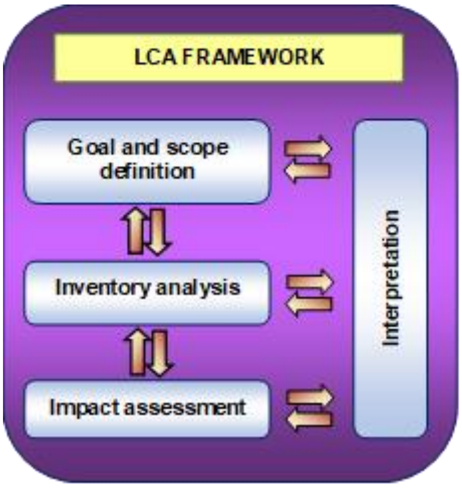


Figure 1: Phases of a life cycle assessment

LCA measures the environmental impacts of economic activities by considering the elementary flows that go from the technosphere to the biosphere or vice versa. To do so, a reference flow, usually represented by the aforementioned functional unit, needs to be defined, which also provides some relevant qualitative and quantitative information regarding the main function of the system (e.g., production of 1 kg of hydrogen at 200 bar and 99.99 %vol of purity). All this information is summarised in the form of matrices within the LCA mathematical framework:

$$\boldsymbol{g} = \boldsymbol{C}\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{f}$$

where *g* is the resulting impact vector, *C* refers to the matrix containing the characterisation factors, *B* refers to the intervention matrix containing all the elementary flows (from the technosphere to the biosphere or vice versa), *A* is the technology matrix describing the flows between economic activities, and *f* stands for the demand vector (20).

LCA has been widely applied to energy systems, including hydrogen-related ones (21,22). The increasing interest in the environmental implications of FCH systems has led to a rise in the number of LCA studies on hydrogen systems, as identified in the review undertaken within the SH2E project (17). Previous projects proposed specific LCA guidelines for hydrogen production/use systems (10,16), thus providing important grounds for the development of the present SH2E guidelines. However, advancements in the field have brought to the surface relevant issues such as the difficulty in comparing environmental results of hydrogen systems (23), the need to consider technology development (24), and other pending methodological issues (17). Within this context, the SH2E guidelines, while being built on the existing ones, identify best practices in LCA of FCH systems and address new topics which are often pending issues not only for FCH-LCA actors but also for the LCA community as a whole.

## 2. Goal of the Life Cycle Assessment

### Motivation

The goal of an LCA establishes the methodological framework capable of correctly answering the questions posed by/to the practitioner. Hence, it strongly influences the whole setup of an LCA, comprising goal and scope, data, and quality assurance. This especially concerns the application situation since LCA is often used for decision support, but can also be found in other applications (19,25). The LCA methodology is application-dependent.

### Description of the topic and key terms

Goal definition is the first step in an LCA. It defines and explains the purpose of the study by answering three main questions related to: (i) expected use of the LCA results, (ii) application situation and reasons for carrying out the study, and (iii) communication strategies (Figure 2). These aspects are strongly linked with each other. All of them have implications in subsequent LCA aspects (e.g., modelling approach and LCI construction) and must be coherent with the practitioner's core question.

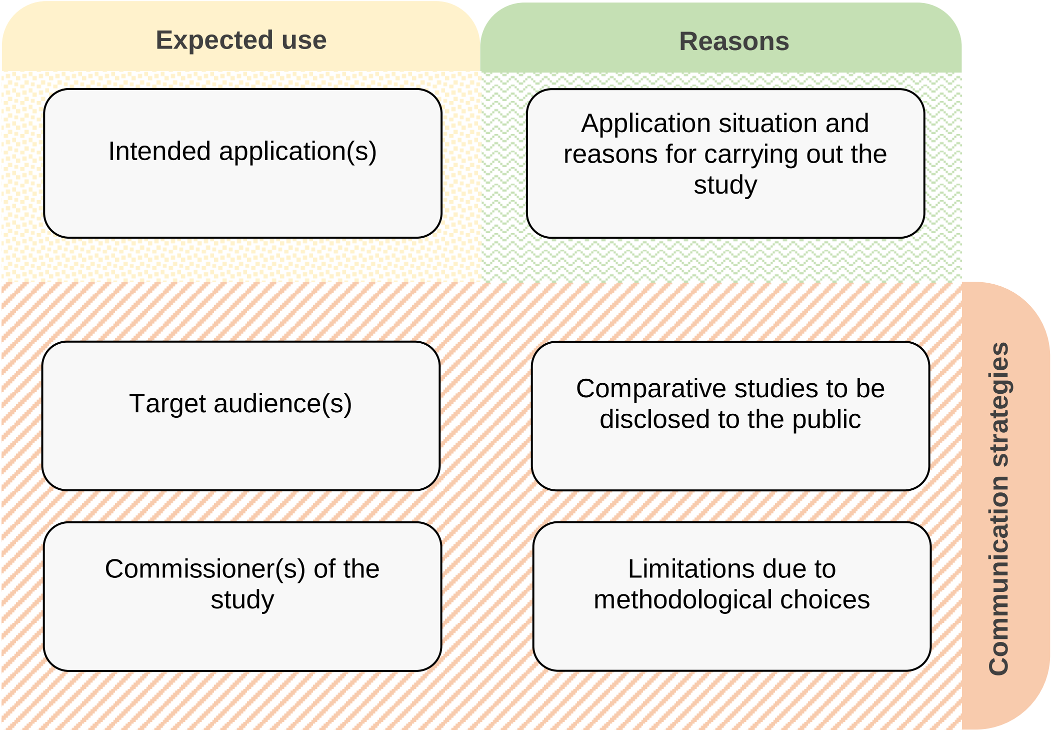


Figure 2: Aspects relevant to the goal definition phase of an LCA

**Intended application(s)**

The expected use of the LCA results could be more than one for a given LCA study. The foreseen applications affect not only the LCA model construction, but also the degree of requirements in terms of verification and data quality. For instance, LCAs intended to guide future policies in the hydrogen sector require a higher degree of verification and data quality than LCAs purely assessing the impacts of a specific product. To reflect these influences and represent the nature of an application, two "dimensions" are proposed:

- Intended reliability, i.e. how reliable do the results need to be:
  - Screening, internal (lowest)
  - Public, non-screening (medium)
  - Policy support (highest)

- Safeground level, i.e. how well the investigated system is known, concerning not only the technology in the foreground system but also supply chains:
    - Retrospective, established technology (highest)
    - Retrospective/current, new technology (high)
    - Prospective, established technology (low)
    - Prospective, new technology (lowest)

More reliable results demand higher levels of verification, and higher data quality. For a system that is well known (i.e., with a higher safeground level), it is easier to achieve higher data quality and to verify the results. However, FCH systems often fall into the prospective / new technology category.

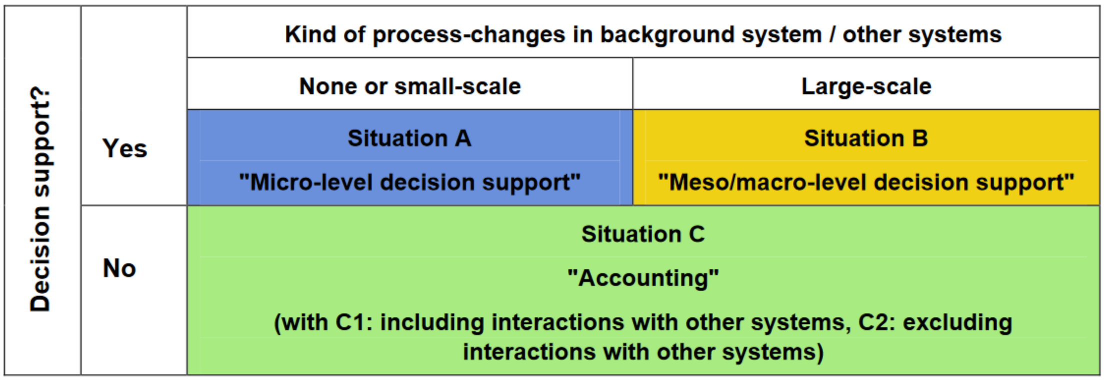
**Application situation and reasons for carrying out the study**

The application situation, also referred to as decision context (16), is intimately linked to the intended application(s) since, depending on the expected use of the LCA results, one modelling approach (e.g., attributional/consequential, retrospective/prospective) may be more appropriate than another (cf. Section 3.1). For instance, in the case of FCH products where a market is yet establishing, an LCA for decision support could be suitable. In such an LCA, the induced change is often not micro but rather at the meso or macro level, and thus an attributional model will often not reflect the changed system in an accurate manner.

Application dependency of LCA has long since been a topic in LCA methodology and LCA guidance. Often, the following “dimensions” are considered:

- Application as decision support or as accounting (19).
- Scale of the decision effect (micro, meso, macro level) (19).

In the ILCD documents, these dimensions lead to the definition of decision situations (Figure 3):



<table>
<tr><td rowspan="4"><b>Decision support?</b></td><td rowspan="3"><b>Yes</b></td><td colspan="2"><b>Kind of process-changes in background system / other systems</b></td></tr>
<tr><td><b>None or small-scale</b></td><td><b>Large-scale</b></td></tr>
<tr><td><b>Situation A</b><br><b>"Micro-level decision support"</b></td><td><b>Situation B</b><br><b>"Meso/macro-level decision support"</b></td></tr>
<tr><td><b>No</b></td><td colspan="2"><b>Situation C</b><br><b>"Accounting"</b><br><b>(with C1: including interactions with other systems, C2: excluding interactions with other systems)</b></td></tr>
</table>

**Figure 3: Decision situations in ILCD** (19)

They are defined as follows (19):

- ***Micro-level decision support:*** *Life cycle based decision support on micro-level, i.e. typically for questions related to specific products. “Micro-level decisions” are assumed to have limited and no structural consequences outside the decision-context, i.e. they are supposed not to change available production capacity.*
- ***Meso/macro-level decision support****: Life cycle based decision support at a strategic level (e.g. raw materials strategies, technology scenarios, policy options). “Meso/macro-level decisions” are assumed to have structural consequences outside the decision-context, i.e. they are supposed to change available production capacity.*
- ***Accounting****: Purely descriptive documentation of the system life cycle under analysis (e.g. a product, sector, or country), without being interested in any potential additional consequences on other parts of the economy.*

Figure 4 indicates how the life-cycle modelling should reflect these different situations (25). The ILCD guidelines (19) recommend attributional LCA for Situation A (micro-level decision support), while they do not detail how the change-oriented LCA that is mentioned for Situation B is to be modelled.

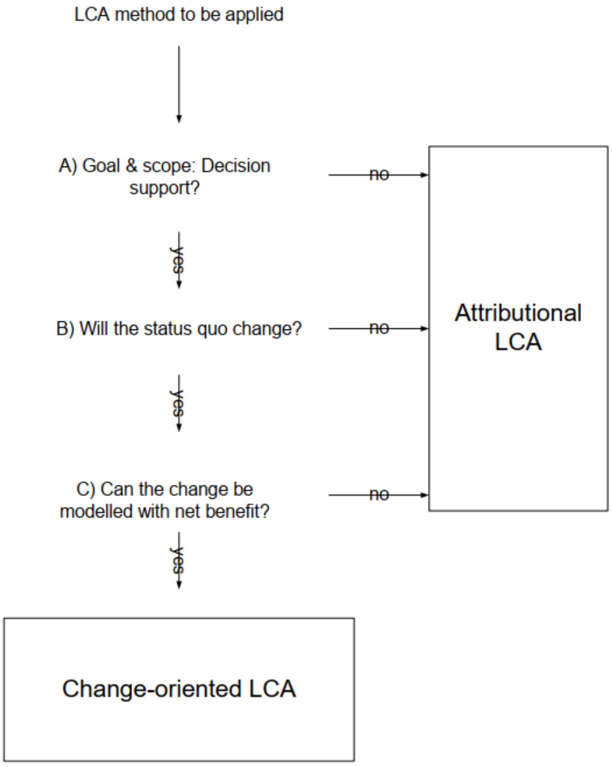


Figure 4: Life-cycle modelling according to decision situation (2)

Together with the two first proposed dimensions (intended reliability and safeground level), these two dimensions (decision support and scale) reflect the entire nature of an application. The interactions between dimensions have some effects that need to be considered by the LCA practitioner when building up the model. Table 1 summarises these issues (verification and data quality are addressed in levels, with 5 being best and 1 being worst):

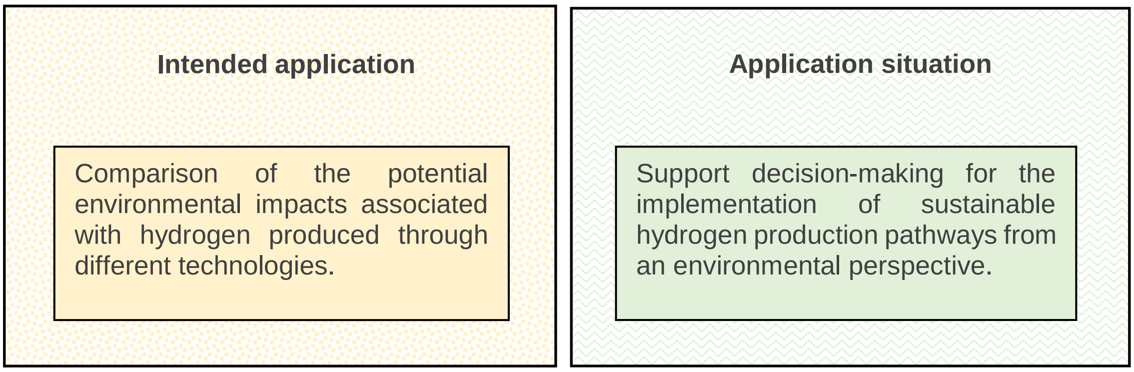
Table 1. Application dependency

| | | **Decision support** | **Intended reliability** | | | | |
|---|---|---|---|---|---|---|---|
| | | no | | | yes | | |
| **Scale** | **Safeground** | Policy support | Public, non-screening | Screening, internal | Policy support | Public, non-screening | Screening, internal |
| meso/ macro | Prospective, established technology | 4;5;5;a | 3;4;4;a | 2;2;2;a | 5;5;5;c* | 4;4;4;c* | 2;2;2;c* |
| | Prospective, new technology | 3;5;5;a | 2;4;4;a | 2;2;2;a | 4;5;5;c* | 3;4;4;c* | 2;2;2;c* |
| | Retrospective / current, new technology | 5;5;5;a | 4;4;4;a | 3;2;2;a | 5;5;5;c* | 5;4;4;c* | 3;2;2;c* |
| | Retrospective, established technology | 5;5;5;a | 5;4;4;a | 4;2;2;a | 5;5;5;c* | 5;4;4;c* | 4;2;2;c* |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **micro** | **Prospective, established technology** | 4;5;5;a | 3;4;4;a | 2;2;2;a | 5;5;5;c* | 4;4;4;c* | 2;2;2;c* |
| | **Prospective, new technology** | 3;5;5;a | 2;4;4;a | 2;2;2;a | 4;5;5;c* | 3;4;4;c* | 2;2;2;c* |
| | **Retrospective / current, new technology** | 5;5;5;a | 4;4;4;a | 3;2;2;a | 5;5;5;c* | 5;4;4;c* | 3;2;2;c* |
| | **Retrospective, established technology** | 5;5;5;a | 5;4;4;a | 4;2;2;a | 5;5;5;c* | 5;4;4;c* | 4;2;2;c* |

| | |
|---|---|
| **first digit:** | verification |
| **second digit:** | data quality background |
| **third digit:** | source transparency and reliability |
| **a:** | attributional LCI modelling |
| **c*:** | change-oriented LCA modelling provided the change is not minor |

As a result of application dependency, an LCA can be modelled as attributional or as change-oriented. Then, verification can be performed more or less thoroughly, and demands on data quality can differ. The data sources used can be of different reliability, and of different transparency. For the sake of clarity, an example showing the required agreement between the *intended application* and the *application situation* is given in Figure 5.



**Intended application**

Comparison of the potential environmental impacts associated with hydrogen produced through different technologies.

**Application situation**

Support decision-making for the implementation of sustainable hydrogen production pathways from an environmental perspective.

**Figure 5: Example of connection between intended application and application situation**

The reasons to carry out an LCA study answer the question *why the LCA study is made* (26). It could also be understood as the core question determining the model prepared to answer it. For instance, a change-oriented LCA would be more appropriate in the example because the goal is to explore the environmental implications of a change at the macro-scale level. The intended application is policy support (highest intended reliability) and technologies with different safeground levels are likely to be involved (e.g., well-established technologies such as SMR and lower TRL production pathways such as high-temperature electrolysis).

### Communication strategies

The aspects to be addressed regarding communication of LCA studies contextualise the LCA results within a specific context of potential readers. It serves to identify the interpretation limits of the study and objectively state the actors involved in the development of the study. Communication strategies are closely linked to the intended application and the application situation since they usually define the target audience of the study. For instance, in comparative studies such as the proposed example (Figure 5), the comparison needs to be stated and high levels of verification would be needed if the study was publicly available (16). The connection with the aspect *Limitations due to methodological choices* is also apparent (26). In the proposed example, an LCA claiming to compare the environmental impacts of hydrogen produced from different technologies should include different impact categories; another limitation could refer to the geographical and temporal scope of the LCA, which could affect, e.g., the efficiency (and therefore the impacts) of the technologies.

## Requirements and recommendations

**Box 1. Intended application of the LCA**

The intended application must be considered for LCAs. The intended application is characterised by the intended reliability and the safeground level. The application situation must be coherent with it, by stating if the LCA study would be employed for decision support (yes/no) and the scale of the induced changes in the considered system (micro, meso or macro).

The nature of the LCA in terms of application situation is determined by its potential use for decision support. Therefore, it is recommended to clearly identify the goal of the study with respect to the economic status quo.

**Box 2. Preferred modelling approach according to the goal**

An LCA that has only the purpose to describe a situation and is not meant for decision support must be modelled following the attributional LCI modelling approach.

An LCA that is meant for decision support needs to follow a change-oriented LCA modelling principle when the anticipated system change induced by the decision at stake is not minor compared to the existing system.

It is recommended to follow the proposed dimensions to characterise the intended application. The quantitative scale given in function of the nature of the application serves as a guideline to efficiently assess data quality and proceed with the verification of the results.

In terms of communication strategies, the practitioner should be as transparent as possible, with especial emphasis on the limitations of the study due to methodological choices. This prevents studies from being inappropriately employed for specific interests by individuals, companies or public institutions.

**Box 3. Limitations of the study**

The LCA practitioner has to clearly state the limitations of the study in terms of use and interpretation of the LCA results. This is even more important when it comes to comparative LCA studies being disclosed to the public.

**Evaluation: “method readiness level”**

- Consideration of the application situation in LCA ●●●●○

**This section is linked to the following sections of the present guidelines:**

- 4.1: Life Cycle Inventory – Data sources and availability
- 4.2: Life Cycle Inventory – Data quality
- 6.2: Interpretation and final remarks – Verification and validation

# 3. Scope of the Life Cycle Assessment

## 3.1 Modelling approach

The choice of the most suitable modelling approach to evaluate the environmental impacts of an FCH product system depends on the **stage of development of the core technology** (technology readiness level (TRL), manufacturing readiness level (MRL), market deployment) and the **goal of the study** (e.g. micro- or macro-level decision; cf. Section 2). Depending on the chosen modelling approach, different foreground and background data sources need to be retrieved from literature or dedicated databases, and the scope of the study also changes in terms of temporal and geographical dimensions, functional unit, methods and impact categories.

The conventional (and widely applied) retrospective approach evaluates the environmental impacts of a product *ex-post* at a present time, i.e. when a product has already been commercialised and used for a time and data are widely available (27). When the core technology is modelled at a future phase, a prospective approach needs to be applied (Section 3.1.1). Depending on the goal of the study, consequential or dynamic modelling can be applied to retrospective or prospective inventories (Figure 6).

For FCH technologies the retrospective approach is largely applied (17). On the other hand, many FCH systems are still at an early stage of development or market deployment, therefore a prospective approach would be recommended despite the challenges in retrieving (generating) reliable inventory data. Additionally, if the study is intended for policy-making, a consequential modelling is recommended, even if very few studies applying consequential modelling on FCH systems appear in the current specific literature (17). The two concepts are thoroughly addressed in this section.

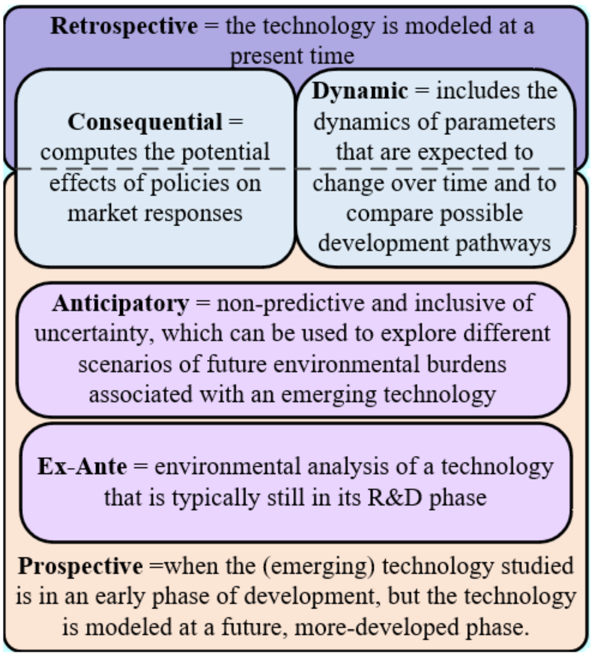


**Figure 6. Classification of forward-looking LCA**

### 3.1.1 Prospectivity

An LCA is defined prospective when **the technology studied is at an early phase of development or market deployment, but it is modelled at a future, more developed phase**. This definition has been adapted from Arvidsson et al. (28) and includes most of the FCH systems. A prospective LCA study is classified as a forward-looking LCA approach along with other non-excluding approaches such as anticipatory or ex-ante LCA (Figure 6) (27).

The approach on how to handle prospectivity in literature is twofold (29):

- Through the inventory by using prospective foreground and/or background data. ●●●●○

- Through the impact assessment method by using prospective characterisation factors. ●○○○○

**Box 4. Prospectivity I**

To be prospective within the context of these guidelines, an LCA study must meet the following requisites:

1. The system must be modelled at a future time. ●●●●●
2. The foreground data for the technical/operating parameters and capital goods of the analysed product system must be prospective. ●●●●●

When performing a comparative study, it must be ensured that the FCH technologies under comparison are modelled at the same future time of implementation.

Additionally, the following recommendations should be considered:

**Box 5. Prospectivity II**

1. The use of relevant prospective background data for processes directly linked to the foreground system (e.g., electricity production) is strongly recommended. ●●●●○
2. The use of prospective background data from dedicated databases (e.g., *premise*) is recommended. ●●●○○
3. It is recommended to state the Technology Readiness Level (TRL) and/or the Manufacturing Readiness Level (MRL) of the involved technology to facilitate comparability decisions.

### Scale effects and learning phenomena in prospective LCA

Prospective LCAs often require the use of laboratory- and/or pilot-scale data, whose direct representativity and comparability with traditional LCA (ex-post or retrospective LCA) data is questionable. The latter refers to mature technologies for which data on large operating scales is widely available, based on years of experience (e.g., SMR). Hence, the consideration of larger operating scales for emerging technologies/market options is needed inasmuch as larger capacities usually imply a reduction in environmental impacts (30). Besides, the improvements a given emerging technology might experience over the years should also be considered. These improvements are known as learning phenomena.

### Recommendations regarding scale and development of FCH technologies in prospective LCA

**Box 6. Accounting for scale effects**

1. Clearly state the assumed operating scale/production capacity.
2. Adapt the life cycle inventory to the considered scale. ●●●○○
3. Account for learning phenomena. ●○○○○

The LCA practitioner should consider two types of phenomena to appropriately assess a technology in the future: (i) scale effects, and (ii) learning phenomena. The former aspect consists in adapting the inventory available for a small-scale system to larger operating scales. The objective is to calculate the inventory data of the assessed system (e.g., energy consumption) on larger operating scales, which are quantified through the corresponding technological parameters of the given system (e.g., power or mass). These relationships apply to the manufacturing life-cycle phase, where economies or diseconomies of scale could appear. The LCA practitioner should identify which inventory flows are independent of the operating scale. The adaptation of the inventory could be done through various methods, including the use of literature values, roadmaps and the adoption of power-law relationships based on empirical data.

**Considering scale in prospective LCA of FCH systems ●●●○○**

The upscaling of a life-cycle inventory to model a hydrogen technology in the future could be done through the use of economic scaling laws as originally postulated for the estimation of equipment capital costs (31). These power-law relationships allow users to account for economies or diseconomies of scale by linking different technological parameters of a system. The power-law formula relates a given parameter of the system ($P_i$) to a known characteristic ($X$), considering a scaling factor ($b_i$) and a normalisation constant ($k_i$). The scaling factor ($b_i$) should be estimated for each of the parameters ($P_i$), being $b_i = 1$ the linear scaling case.

$$P_i = k_i \cdot X^{b_i}$$

Data points should be available for $P_i$ and $X$, checking whether a statistically significant relationship exists between the two parameters. The common approach used to determine $b_i$ and $k_i$ is to apply ordinary least linear regression on the log-transformed data. Examples of this procedure can be found in (30).

$$log(P_i) = \log(k_i) + b_i \cdot \log(X)$$

Once the analysis is done, the property $P_i$ for the new scale can be derived from the technological characteristic $X$.

Learning phenomena refer to the improvements a technology experiences over time due to the accumulated knowledge of its scientific principles and production processes, and the gradual improvement of its manufacturing process. This definition responds to both types of learning phenomena: learning-by-searching and learning-by-doing (32). It was originally applied to estimate the cost per unit of a product, although it could be applied to study the evolution of technological parameters. The consideration of learning phenomena in prospective LCA allows practitioners to appropriately evaluate the environmental performance of hydrogen systems and make fair comparisons. For instance, mature hydrogen systems have already benefited from some of these effects, optimising their conception and manufacturing. Learning phenomena could be sometimes difficult to quantify, especially for low-TRL technologies, because of limited data availability regarding accumulated production. It could be expressed through different models. However, it is not simple to disaggregate learning phenomena from economies-of-scale effects. The common approach in LCA is to quantify both mechanisms together through the use of experience curves.

**Considering learning phenomena in prospective LCA of FCH systems ●○○○○**

Experience curves, applied to a life-cycle inventory, link the property of interest at the time assumed for the LCA model with the cumulative production at that time in the future. To do so, power-law relationships are also employed. Experience curves take into consideration both effects, economies-of-scale and learning mechanisms. Following the nomenclature in (30), the scaling factor ($b_i$) is transformed into the experience index ($z_i$). $P_{i,c}$ corresponds to the key parameter at the cumulative production $C$, while $P_{i,o}$ is the current value considered for the $P_i$ parameter at the current cumulative production $C_0$.

$$log(P_{i,c}) = \log(P_{i,o}) + z_i \cdot \log(C/C_0)$$

Information on learning rates can be available. According to the original definition of learning curve (33), the learning rate ($LR$) is defined as the rate at which the property ($P_i$) decreases when the cumulative production is doubled.

$$LR = 1 - 2^{z_i}$$

As for the inventory scaling, the LCA practitioner must study whether linear correlations are statistically significant so as to select the correct parameters ($P_i$). Note that experience curves may be applied independently of the scaling, since they capture two mechanisms linked with a higher production volume and experience.

**Technology maturity**

While the TRL is used to represent the maturity of an individual technology, the MRL is used to express the maturity of a given technology, system, subsystem or component from a manufacturing perspective. In the context of prospective LCA of FCH systems, both parameters are relevant. Indeed, many FCH products are commercial (high TRL) but their industry is not fully deployed or their market penetration is still limited (low MRL). In this case, attention must be paid in prospective LCA when considering scale effects and learning phenomena. A tentative list of FCH technologies and their TRL is reported in Table 2. Reliable information on the MRL of the technologies is usually scarce, but, whenever possible, it is recommended to take it into consideration and clearly state it in the study.

Table 2. FCH technologies and their TRL

| Stage | FCH technology | TRL | Reference |
|---|---|---|---|
| *Production* | Steam methane reforming (SMR) | 9 | (34) |
| | Coal gasification | 9 | - |
| | Partial oxidation of mineral oil products | 9 | - |
| | Biomass pyrolysis and gasification | 8 | (34) |
| | Raw biomass reforming | 9 | (34) |
| | Thermochemical water splitting | 3-6 | (34,36) |
| | Photocatalysis | 2-5 | (34) |
| | Fermentation (biological $H_2$ production, dark fermentation) | 4 | (34) |
| | Supercritical water gasification of biomass | 4 | (34) |
| | Photo-biological water splitting including algae bioreactors and photosynthetic microbes | 1 | (34) |
| | Photofermentation | 3 | (34) |
| | Electrohydrogenesis | 1 | (34) |
| | Plasma-supported gasification | 9 | (34) |
| | Plasma-based carbon black process | 4 | (34) |
| | Alkaline electrolyser (AEL) | 9 | (35,36) |
| | Proton exchange membrane electrolyser (PEMEL) | 6-8 | (35,36) |
| | Solid oxide electrolyser (SOE) | 5-7 | (35,36) |
| *Compression* | Turbo compressors | 9 | (37) |
| | Piston compressors | 9 | (37) |
| | Membrane compressors | 9 | (37) |
| | Ionic compressors ($H_2$ filling stations) | 7 | (37) |
| | Electrochemical compressors | 3 | (37) |
| *Storage & transport* | Gasometers (up to 1 bar) | 9 | (37) |
| | Pipe storage (up to 100 bar) | 9 | (37) |
| | High-pressure hydrogen storage cylinders (up to 700 bar) | 8-9 | (38) |
| | Cavern storage | 8 | (37) |
| | Pore/aquifer storage | 3 | (37) |
| | Fuel tanks for cryo-compressed $H_2$ for mobility | 6 | (37) |
| | Metal hydrides | 4-9 | (38,39) |
| | Liquid organic hydrogen carriers (LOHC) | 5-7 | (37) |
| | Liquid hydrogen/adsorption materials | 4-6 | (37,39) |
| | Tanks for liquid hydrogen | 9 | (37) |
| | Magnetic cooling | 3 | (37) |
| | Slush hydrogen | 3 | (37) |

**Table 2. FCH technologies and their TRL (continued)**

| Stage | FCH technology | TRL | Reference |
|---|---|---|---|
| *Use* | Hydrogen internal combustion engine | 8 | (39) |
| | Alkaline fuel cell (AFC) | 7-9 | (40) |
| | Proton exchange membrane fuel cell (PEMFC) | 8-9 | (41) |
| | Solid oxide fuel cell (SOFC) | 4-8 | (41) |
| | Molten carbonate fuel cell (MCFC) | 7-9 | (37,41) |
| | Phosphoric acid fuel cell (PAFC) | 7-9 | (37) |

### 3.1.2 Consequentiality

Also called *change-oriented* or *effect-oriented LCA*, the consequential LCA approach was first introduced in the 1990s (42). Many definitions were given over the years. According to the UNEP/SETAC definition, it attempts to provide information on the environmental burdens that occur, directly or indirectly, as a consequence of a decision (usually represented by changes in demand for a product) (11). In other words, the consequential approach aims at quantifying how environmentally-relevant flows and impacts of a product system may change in response to a change of production volumes or demand.

In contrast to the attributional approach, which uses average data and may apply allocation to deal with multi-functional systems, the consequential approach uses data of actual suppliers or marginal technology data and deals with multi-functionality by using system expansion to include the processes affected by the consequences of the change (11,43). One of the most critical aspects is the identification of the processes that are affected by the change, as well as the need to guarantee the functional equivalence between the systems under evaluation in comparative assessments. These aspects are partially addressed by Zamagni et al. (44) and Earles and Halog (45). Currently, technological data in consequential LCAs are assumed equal or very similar to current processes, which constitutes a strong assumption especially when referring to long-term horizons.

In contrast to attributional LCA, consequential LCA can be applied for decision-making at macro-scale (46,47). Currently, consequentiality in LCI is mainly addressed through three different approaches:

- Expert data (also for the previous identification of marginal technologies).
- Dedicated databases with marginal technology data (after separate identification of marginal technologies).
- Economic modelling (also for the previous identification of marginal technologies).

The introduction of market mechanisms in the analysis is a key aspect in consequential LCA. The common supply and demand mechanisms introduce perturbations in the system, giving rise to a chain of cause-effect relationships. These market mechanisms are derived from economic models or outlooks in specific sectors, and then included as input in the assessment (44). While initial efforts relied mainly on simple partial equilibrium (PE) models and heuristic approaches for determining affected technologies, more recent techniques incorporate sophisticated economic models for this purpose (e.g., multi-market multi-regional partial equilibrium models and computable general equilibrium models) and consider economic notions such as rebound effects and experience curves (45).

The following broad classification of consequential LCA models applies (48):

- **Linear production models:** process-based and input-output based LCA.
- **Non-linear optimisation models:** computable general equilibrium (CGE) models.

The first approach refers to linear models which use linear extrapolation to approximate changes. Besides, the impact associated with a change of demand is a linear function of the change of demand itself. These models rely on several assumptions, such as the use of constant input/output coefficients (i.e., no economies/diseconomies of scale or capacity effects are applied). Furthermore, it is assumed that there is infinite potential of supply for inputs and an infinite market capacity to assimilate additional products.

The second approach was created to include in the modelling important characteristics of the market, such as substitution, price effects, elasticity of supply and demand, and rebound effects. Despite accounting for sophisticated flow-price relationships, non-linear models involve important assumptions, e.g. regarding the choice of parameters and functional forms and standard neoclassical economic assumptions such as the assumption according to which individuals have rational expectations and maximise utility and industries maximise profits.

Overall, each of the models has its own strengths and weaknesses according to particular applications. In fact, models can be complementary rather than contradictory (49), so the choice of the model to be applied ultimately depends on the research question and the considered time horizon. Besides current limitations of consequential LCA, the choice of the modelling approach (attributional or consequential) depends on the purpose of the study (Section 2).

### Requirements and recommendations

While a full specification of guidelines for consequential LCA of FCH systems is beyond the scope of this document, some general recommendations are given.

**Box 7. Consequentiality I**

If the LCA study is aimed at a macro-level decision (e.g., policy-making), a consequential approach has to be followed.

**Box 8. Consequentiality II**

1. The identified marginal technologies should be clearly stated and reported, including a justification on the choice of the marginal technologies and the procedure followed for that identification.
2. The quantification of the change in marginal technologies should be clearly stated, reported and justified, clearly specifying the procedure followed for that quantification.
3. The quantification of the environmental impacts of the change should be clearly reported (data sources, procedure, results, etc.).

Besides that, the following recommendations apply:

4. Whenever an economic model is applied, the user should give full traceability of the economic models/equations applied and the input data used for the study.
5. A clear statement of the time horizon of the consequences (short, medium, long term) is recommended.
6. Whenever a consequential approach is needed, it is recommended to evaluate results for different models, especially if applied in the context of policy-making.

**Application of consequential modelling to FCH systems**

Literature currently lacks extensive application of consequential LCA to FCH systems. In particular, between 2012 and 2020 only four examples of consequential modeling applied to FCH systems were published (17,21). Despite its limited use, consequential LCA could play a key role regarding macro-level decision for emerging technologies that are forecasted to achieve a high market penetration, such as FCH systems.

Previous applications of consequential LCA to FCH systems include: penetration of hydrogen technologies in the Orkney islands (50), analysis of the economic and environmental impacts caused by the penetration of FCEVs in Germany in 2050 (51), and evaluation of the environmental impacts of substituting diesel and gasoline vehicles with FCH technologies in Taiwan for different scenarios of hydrogen production (52,53). Each of the aforementioned papers uses different methodologies to model consequentiality. Zhao et al. (50) built a linear consequential model, while Rocco et al. (51) proposed an approach based on a linear *hybrid integrated input-output analysis*. Finally, Chen et al. (52,53) proposed a *graphical representation* to model consequentiality.

The few examples found in the literature for FCH systems are hereby mentioned only for reporting purposes, while the present LCA guidelines do not support or discourage any of the applied methodologies.

**This section is linked to the following section of the present guidelines:**

- 2: Goal of the Life Cycle Assessment

## 3.2 Functional Unit

### Motivation

The **functional unit** of an LCA represents the principal function of the system under study, according to the goal and scope of the LCA (1). It corresponds to a **reference flow** to which all the inputs and outputs of the system are related (1,54). The functional unit is, therefore, a quantitative representation of the main function of the system. In the case of systems providing more than one function (**multi-functional systems**), the practitioner must isolate/choose one of the functions since LCA results are related to a single reference flow (54). Besides, special attention should be paid when carrying out **comparative LCAs** because the functional unit must represent a common function accomplished at the same level (e.g., hydrogen produced with the same degree of purity and with the same final temperature and pressure).

According to the review performed within the scope of the SH2E project (17), LCA studies of FCH systems present three main particularities regarding functional unit definition: heterogeneity of the **reference flow** for a given functional unit, high occurrence of **multi-functional systems**, and **benchmarking purpose**. These three topics need to be taken into account to ensure a correct choice of the functional unit. Besides, the review performed showed new trends concerning the functional unit definition compared to a previous review (21), revealing that a certain degree of scientific consensus has already been achieved (17). This section seeks to propose general recommendations for functional definition in LCAs of FCH systems.

## Description of the topic

Hydrogen may be involved in a great variety of supply chains (e.g., electricity, fuels, chemicals), and might appear at different stages of the life cycle. It could be employed as a fuel itself or used to fulfil another function such as energy storage and chemicals production (e.g., ammonia and methane). This versatile nature allows hydrogen to provide very different functions, which results in the need to define functional units of different sort (17). Therefore, it is crucial to identify which is the **main function of the system** and define the functional unit accordingly. In addition, many hydrogen systems are identified as multi-functional ones. For example, the chlor-alkali process could have three main functions: chlorine, sodium hydroxide, or hydrogen production; corresponding to its three **functional flows.**

Because of the great heterogeneity observed regarding hydrogen uses, this section differentiates between **systems exclusively assessing hydrogen production, and those including its use within the system boundaries**. This disaggregation leads to more concrete recommendations, and it is in line with the system boundaries observed for LCAs of FCH systems (Section 3.3).

## Options

Different cases are herein distinguished for functional unit definition:

- **Case 1**: Systems exclusively assessing hydrogen production.

- **Case 2**: Systems including hydrogen use within the system boundaries:
  - 2a. Hydrogen for transportation.
  - 2b. Hydrogen for fuels and chemicals production.
  - 2c. Hydrogen for electricity and/or heat generation.

## Requirements and recommendations

### General recommendations

The first step is to identify the function of the system that wants to be assessed (Box 9). This could be straightforward in the case of systems with a single functional flow or a clear goal. For systems with various functional flows (multi-functional systems), the LCA practitioner should identify the functional flows as recommended in Section 3.4. This identification serves to consider alternative functions of the system and recognise co-products. Once the functional unit has been selected, the functional flow serving as reference flow of the system must be identified and quantified.

**Box 9. Identification of functional unit, functional flows and reference flow**

1. The function of the system to be assessed must be identified.
2. The functional flows of the system, if more than one, must be identified and reported to clearly state the methodology employed for their handling later on (Section 3.4).
3. The reference flow of the system must be indicated and quantified.

In some situations, the identification of the main function of the system may present some difficulties because of the use of hydrogen as an **energy vector**. The LCA practitioner should be aware that hydrogen can act as an energy transportation or energy storage media. For example, employing renewable electricity surplus to produce hydrogen through electrolysis may have as main goal the production of hydrogen, or just the storage of renewable electricity. The identification of the function of the system is given by a qualitative analysis by the LCA practitioner, who needs to evaluate whether the goal of the system is to produce hydrogen or to store renewable energy. This discussion is more significant when developing comparative studies because equivalent functions are required. In the case of comparative LCAs, the functional unit must guarantee that the function of the systems is the same. Attention should also be paid to analyse whether all the systems achieve the minimum level of qualitative requirements set for the function (Box 10) (54). These qualitative considerations are set by the LCA practitioner depending on the goal of the system (e.g., hydrogen threshold purity for its usage in fuel cells). A clear definition of the qualitative characteristics that the product should attain is key to ensure a fair comparison between different systems. Variations in the reference flow quantity could arise if there are differences in quality or performance among the different systems assessed.

**Box 10. Functional unit in comparative LCAs**

1. Comparative LCAs must ensure that the selected functional unit represents the common function of the systems and allows a fair comparison.
2. Qualitative considerations to be achieved by the evaluated systems, which can be made in the form of quantitative thresholds or qualitative statements, must be clearly defined.

**Requirements and recommendations for Case 1: Systems exclusively assessing hydrogen production**

Regardless of the assessed hydrogen production pathway, there has been a shift in literature towards the adoption of a common functional unit for hydrogen production (17). The mass of produced hydrogen was selected as the functional unit in all the reviewed case studies (17), proving that there is a general scientific agreement in this sense (which could be related to harmonisation initiatives such as the IEA Hydrogen Task 36 (55)). This agreement was not identified in a previous review (21), nor in previous hydrogen guidelines (16). Differences regarding the recommended functional unit also arise when assessing hydrogen according to the regulatory methodological framework available in the Renewable Energy Directive on the promotion of the use of energy from renewable sources (RED II) (56). Therefore, the recommendation given in the SH2E guidelines is to state the functional unit as a description of the produced hydrogen amount (16). Considering literature trends and regulatory frameworks, it is proposed to use the **mass of produced hydrogen or the energy output in terms of hydrogen** (Box 11). For the latter, the **net calorific value** (NCV; also known as lower heating value, LHV) of hydrogen must be stated.

The functional unit must in all cases be accompanied with a **proper definition of the reference flow**. As also pointed out in previous FCH-specific LCA guidelines (16), **hydrogen purity, pressure and temperature** must be stated together with the quantity of produced hydrogen (Box 11). These characteristics are linked to important life-cycle stages such as compression and purification and affect hydrogen properties such as the NCV, being especially crucial in comparative LCAs.

### Box 11. Functional unit in systems assessing hydrogen production

1. The functional unit employed in LCA of hydrogen production systems must represent the quantity of produced hydrogen by means of a mass- (**kg of hydrogen**) or energy-based (**MJ of hydrogen**) functional unit.
2. In the case of employing an energy-based functional unit, the energy content of hydrogen must be clearly stated through the specification of the **net calorific value** (lower heating value).
3. **Hydrogen purity, pressure and temperature must be specified** together with the functional unit to guarantee a precise functional unit and fair comparisons.

The precise description of the reference flow was identified as one of the main gaps in LCAs of hydrogen systems (17). Therefore, it is recommended to include the reference flow in the initial flow diagram of the LCA (Section 3.3). This also serves to indicate which is the reference flow in the case of multi-functional systems.

### Box 12. Reference flow in systems assessing hydrogen production

The reference flow, completely defined through the specification of hydrogen purity, pressure and temperature, should be indicated in the initial flow diagram of the LCA.

#### Requirements and recommendations for Case 2: Systems including hydrogen use within the system boundaries

The heterogeneity of hydrogen applications claims for different functional units with the aim of correctly representing the function of the system. Considering that new applications for hydrogen may appear in the short and long run, this section makes general methodological recommendations. It is useful to differentiate between the system and subsystem functions. If the FCH section is a part of a larger system (for example, power production in a transportation system), a difference should be stated between the main system and subsystem functions (57). Some current applications, which already have a certain level of technological development, are highlighted below. Nevertheless, LCA practitioners interested in assessing potential future applications could still follow these methodological recommendations, along with the suggestions made in Section 3.1.1 concerning prospective LCA.

#### Case 2a. Hydrogen for transportation

The most assessed application of hydrogen is hydrogen use as a fuel for transportation (17). There is a general agreement on following distance-based functional units (km, pkm, tkm) depending on the specific goal of the study. The choice of a **distance-based functional unit is therefore required** (Box 13) since it also allows for an easy comparison with other powertrain technologies. The specific functional unit to be selected depends on the goal of the LCA, but a proper definition of the reference flow must be included, reporting capacity utilisation (passengers/transported freight) and the lifetime considered for the vehicle in terms of mileage. For example, the reference flow could be stated as “to travel X km with a fuel cell electric vehicle of medium size (Y kg) occupied by Z passengers with an expected lifetime of W km”. The specific reference flow may include other characteristics according to the goal of the LCA, but the relationship between distance and demand (in the form of load) must always be clear. This statement is not limited to road transport but it also includes other modalities such as air and maritime transportation.

### Box 13. Functional unit in systems assessing hydrogen use for transportation

1. The functional unit employed in LCAs of hydrogen use for transportation must **represent the distance travelled for a given demand**, expressed as the passenger or freight load.
2. The considered demand must be specified in the reference flow, together with the lifetime measured in terms of mileage.

### Case 2b. Hydrogen for fuels and chemicals production

Hydrogen is employed in multiple processes for the synthesis of chemicals and fuels. The main applications foreseen are **methane, methanol, and ammonia production**. A functional unit that describes the produced amount must be employed (Box 14). The reference flow is to be specified stating the **purity, pressure and temperature of the produced chemical/fuel**. In the case of fuels, it is also necessary to report the NCV of the resulting fuel.

### Box 14. Functional unit in systems assessing hydrogen use for fuels and chemicals production

1. The functional unit employed in LCAs of hydrogen use for fuels and chemicals production must **represent the quantity of the produced chemical/fuel** by means of a mass-based functional unit in the case of chemicals, and by either a mass- or energy-based functional unit in the case of fuels.
2. **Purity, pressure and temperature of the produced chemical/fuel must also be specified** to guarantee a precise functional unit and fair comparisons.
3. In the case of fuels, the energy content must be clearly stated through the use of the

### Case 2c. Hydrogen for electricity and/or heat generation

Systems using hydrogen as a fuel for energy generation could be classified into: electricity generation, and cogeneration. The formers are conceived for the production of a single product (electricity), which is the only functional flow of the system. The function of these systems is clear and an **energy-based functional unit** is commonly employed (17), a trend previously identified in literature (21). This energy-based functional unit must refer to the **output electricity** (Box 15); thus, it **considers upstream efficiencies** (engine or fuel cell, rectifier for fuel cells, and generator). It is recommended to include and clearly state the upstream efficiencies to be able to retrieve the reference flow of the system.

### Box 15. Functional unit in systems assessing hydrogen for electricity and/or heat generation I

The functional unit employed in LCAs of hydrogen use for electricity generation must represent the quantity of produced electricity (MJ or equivalent). The functional unit must consider the upstream efficiencies to convert hydrogen into electricity.

For cogeneration systems, two functional flows appear: electricity and heat. The LCA practitioner should determine if heat is considered as a valuable product (functional flow) or, when not used, an emission to the environment. For the latter, the system would only be producing electricity and should follow the recommendations given in Box 15. On the contrary, when heat is a valuable product, the function of the system changes because it becomes “the production of electricity and heat”. This combined function should be represented by an **exergy-based functional unit**, which represents the maximum energy potential that the system could transform into useful work (Box 16).

### Box 16. Functional unit in systems assessing hydrogen for electricity and/or heat generation II

The functional unit employed in **LCAs of hydrogen use for electricity and heat generation must represent the maximum energy potential** that the system could transform into work (i.e., exergy-based functional unit).

If heat is considered as a valuable product of the system, it is not recommended to apply allocation for comparative purposes since cogeneration would be the actual function of the system. Hence, the system should be benchmarked with functionally-equivalent systems such as combined heat and power (CHP) engines rather than addressing a separate benchmarking of each product.

**This section is linked to the following sections of the present guidelines:**

- **3.1.1: Scope of the Life Cycle Assessment – Modelling approach – Prospectivity**
- **3.3: Scope of the Life Cycle Assessment – System boundaries**
- **3.4: Scope of the Life Cycle Assessment – Multi-functionality**

## 3.3 System Boundaries

### Motivation

The system boundaries of a Life Cycle Assessment (LCA) are a set of criteria that specify which processes are included in the product system and therefore determine which unit processes shall be included in the LCA. The system boundaries shall be consistent with the chosen goal of the LCA (1). The correct identification and reporting of the chosen system boundaries are crucial, especially in the case of comparative studies.

Concerning FCH systems, a **lack of transparency regarding the flows included in the system boundaries** still persists (17), which often causes problems during comparison and benchmarking. Most of the studies include capital goods, while very few include the end-of-life (EoL) and, if so, few details are reported and a clear identification of the EoL scenarios is missing. Another specificity of FCH systems is the large variety of life-cycle phases where the study boundary might be placed, especially in studies assessing hydrogen production. In fact, after being produced, hydrogen undergoes conditioning (purification and compression), storage, transportation, and distribution before reaching the use phase. The choice of the gate largely varies depending on the specific study (Figure 7). The setting of the system boundaries in LCA of hydrogen systems is key to ensure that the desired reference flow is achieved and, therefore, the function of the system performed.

### Options

Different cases are herein distinguished for the system boundaries definition:

- **Case 1**: hydrogen production.
- **Case 2**: hydrogen use.
- **Case 3**: hydrogen production and use.

For case studies focusing on FCH technology manufacturing, the operational phase of the technology should be included. By doing so, this case study should match one of the three cases before.

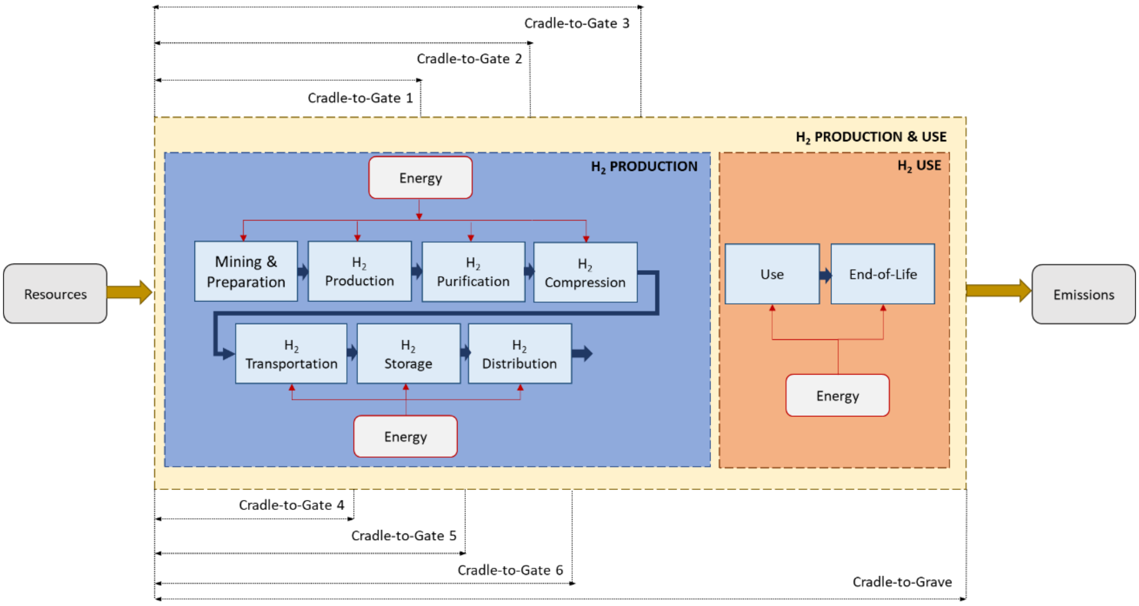


Figure 7. System boundaries for studies assessing FCH systems

## Requirements and recommendations

### General requirements and recommendations

**Box 17. System boundaries I**

1. The system boundaries definition has to be coherent with the goal of the study.
2. The system boundaries of the analysed system must be defined and reported.
3. The system boundaries have to include the capital goods life cycle, including their EoL, with an appropriate reporting of the latter (cf. Section 3.3.2).

**Box 18. System boundaries II**

1. The use of any cut-off is discouraged. When applied, it must be clearly stated and justified.
2. It is highly recommended to show the system boundaries in a flow chart.

### Requirements and recommendations for Case 1: hydrogen production

When conducting LCA studies assessing only hydrogen production, the recommended system boundaries are cradle-to-gate, including hydrogen conditioning (Cradle-to-Gate 3 in Figure 7). This recommendation assures that the produced hydrogen could fulfil the function of the system (e.g., provide high-purity hydrogen for FCEVs). The reference flow definition, which involves hydrogen specifications and thermodynamic conditions (e.g., pressure, temperature, purity), might vary depending on the goal of the study and the intended application. Regardless of the final gate chosen for the assessment, these aspects need to be clearly specified and reported (cf. Section 3.2).

### Box 19. System boundaries for systems assessing hydrogen production I

1. The system boundaries of studies on hydrogen production have to be, at least, **Cradle-to-Gate 1**.
2. All the relevant flows, according to the environmental indicators subject to assessment, have to be included in the assessment. If any is disregarded, it must be reported and justified.

### Box 20. System boundaries for systems assessing hydrogen production II

1. It is recommended to place the gate after the hydrogen conditioning section, in particular after the compression stage (Cradle-to-Gate 3).

### Requirements and recommendations for Case 2: hydrogen use

For studies focusing on hydrogen use, it is required to assess the product life cycle from resource extraction to the use and disposal phase (i.e., Cradle-to-Grave). This means that hydrogen production has to be included in the analysis, checking that the considered hydrogen is suitable (purity and pressure) for the assessed application and methodologically consistent. In this sense, directly implementing literature results for the life-cycle impacts of the produced hydrogen is not recommended (i.e., using previous life-cycle results to account for the production phase when performing a cradle-to-grave study on hydrogen) Additional aspects should be considered concerning the LCA scope and the scale of the system to avoid the implementation of environmental burdens that do not necessarily fit the time of modelling and/or scale of the assessed hydrogen use. It should be noted that the case where hydrogen production is modelled by the user falls into Case 3 (hydrogen production and use).

### Box 21. System boundaries for systems assessing hydrogen use

1. The system boundaries of studies focusing on hydrogen use have to be **Cradle-to-Grave**.
2. All the relevant flows, according to the environmental indicators subject to assessment, have to be included in the assessment. If any is disregarded, it must be reported and justified.

### Requirements and recommendations for Case 3: hydrogen production and use

When conducting an LCA of systems for hydrogen production and use, cradle-to-grave studies are required, including capital goods and EoL (cf. Sections 3.3.1 and 3.3.2).

### Box 22. System boundaries for systems assessing hydrogen production and use

1. The system boundaries of studies on hydrogen production and use have to be **Cradle-to-Grave**.
2. All the relevant flows, according to the environmental indicators subject to assessment, have to be included. If any is disregarded, it must be reported and justified.

**This section is linked to the following sections of the present guidelines:**

- 3.2: Scope of the Life Cycle Assessment – Functional Unit
- 3.3.1: Scope of the Life cycle Assessment – System boundaries – Capital goods
- 3.3.2: Scope of the Life cycle Assessment – System boundaries – Equipment end-of-life

### 3.3.1 Capital Goods

In order to produce goods or provide services, different **physical items** are necessary **to enable the producer to manufacture the product**. At this point of production systems, the so-called **capital goods** come into effect (58). Even though the **classification of system components as capital goods depends on the perspective** of the particular study (59), they can be described with components like machinery used in production processes, buildings, office equipment, transport vehicles, and transportation infrastructure (4). In fact, physical items that are usually labelled as **“capital goods” may become the focus of LCA studies** and thus lose their “capital goods” classification in the sense of this guidelines section. The described requirements and recommendations are still valid in such cases for capital goods needed to provide these focused products.

Capital goods (e.g. electrolyser, compressors, etc.) **have to be included** within the system boundaries (14), as an exclusion could lead to misleading results (60). Capital goods cannot be excluded per se and should be treated as any other input or output flow (58,59).

Since the usage duration often exceeds the relevant considered period of the studied goods or services, **capital goods’ lifetime has to be taken into account by linear depreciation** (4). This specifically does not include the economic amortisation period, but their effective service life. Besides the production and use of capital goods, the related **EoL activities** (cf. Section 3.3.2) **shall be considered**.

For reasons of transparency and completeness, **documentation regarding capital goods consideration** has to be added to the reporting. Essential information are data sources and made assumptions.

**Box 23. Capital goods I**

To conduct LCA studies in line with these guidelines for FCH systems, the following **requirements shall be fulfilled**:

1. Capital goods have to be included by their phases of production, use and EoL. ●●●●●
2. The non-consideration of capital goods shall be justified by cut-off rules. ●●●●○
3. The effective lifetime of capital goods has to be included. ●●●●○
4. Data sources and assumptions related to capital goods shall be documented. ●●●●●

As in the case of the other parts of the system under investigation, in the case of capital goods the **use of qualitatively appropriate data is also recommended** to increase reliability and robustness of the study. This appropriateness includes the framework on data quality requirements defined in Section 4.2.

For the sake of rigour and considering data availability, it is **recommended to use data with the same geographical and temporal reference for capital goods as for the other parts of the system**. This can prevent potential result-distorting influences of technology development, for example.

**Capital goods can contribute substantially to specific categories**, for example human toxicity, resource criticality, and land use (58,61). For a better classification of results, it is recommended to take a closer look on the influence of capital goods on specific categories.

**Box 24. Capital goods II**

When considering capital goods in LCA studies in line with these guidelines for FCH systems, the **following points are recommended**:

1. Depending on data availability, it is recommended to use qualitatively appropriate data. ●●○○○
2. The geographical and time horizons considered for the capital goods should be consistent with the data employed for the rest of the life-cycle phases. ●●●○○
3. The influence of capital goods on certain impact categories should preferably be highlighted in the reporting. ●●●○○

Regarding the **identification or determination of capital goods**, the specific components will differ depending on the study objective. Additional documentation including the labelling of such components by the LCA practitioner facilitates the understanding.

**Capital goods identification and perspectives**

A systematic listing of relevant components for hydrogen production and/or use systems eases the identification of capital goods. To get a general idea of the components to be potentially included in the identification approach, an **exemplary visualisation of components** in the context of EoL is given in Valente et al. (62). They show EoL strategies at the technology level illustrating the technical structure of PEMFCs (proton exchange membrane fuel cells), SOFCs (solid oxide fuel cells), PEMWEs (proton exchange membrane water electrolysers), and AWEs (alkaline water electrolysers) and dividing them into stack and BoP (balance-of-plant) components as well as exemplary relevant subordinate units.

Additionally, Valente et al. (63) offer an **exemplary orientation on capital goods** in the context of cumulative energy demands for renewable hydrogen production. The listed items to be classified as capital goods are electrochemical, biological or thermochemical plants related to hydrogen production and conditioning, for example. Regarding electricity production, fossil, nuclear, and renewable plants are listed as capital goods.

These publications rather take the viewpoint of a plant operator or hydrogen-production-equipment manufacturer and thus define the objective of the related study and the capital goods with a specific approach. However, the **perspective of an LCA practitioner may differ depending on the goal of the assessment**. For example, if the study on hydrogen production or use is designed from the position of a manufacturer of hydrogen storage tanks, the production of these tanks will not be under the heading of capital goods. Even though hydrogen tanks are capital goods, they would be subject to special attention by the manufacturer for reasons of interest. Accordingly, the **identification of capital goods always requires a defined perspective** of the LCA study.

### 3.3.2 Equipment End-of-Life

An important topic with regard to the system boundaries is the consideration and handling of products at the end of their life. Thus, **EoL is an integral component of the product life cycle** and shall be included in LCA modelling (14,64,65). The following general definition and description of the EoL is based on definitions in different publications and guidelines (64,66–68):

*The beginning of the EoL can be defined as the point at which a* ***product stops its function or reaches a point of critical diminishing usability****, so that the* ***consumer or user is no longer satisfied with or discards the product****. EoL describes the final stage of a studied product system. During the EoL stage, materials or components of the former product* *undergo an EoL treatment and return to environment (disposal) or enter another or new product life cycle (reuse, recovery, recycling).*

The end of the EoL is given when a **specific flow crosses the system boundary to leave the product system (waste) or enter a new/another life cycle** (61). Depending on the flow and EoL modelling (cf. box “*EoL modelling methods*”), this endpoint can differ. In the case of including recycling or recovery processes, this point, which is usually known as point of substitution, is reached with the “outflow of recovered/recycled material” (69). Figure 8 illustrates the general product life-cycle stages and contained activities.

EoL can lead to multi-functionality in the system (14,64,69), which should be addressed in accordance with Section 3.4. Thus, allocation should be avoided by system subdivision or expansion also in the EoL modelling (14,64,69). The modelling of EoL varies depending on the applied approach (box “*EoL modelling methods*”). The **choice of the method has to be documented** by the LCA practitioner and **requires justification**.

Regardless of the EoL flows fate (disposal, recycling, recovery or reuse), **preparatory steps before the core EoL treatment** shall be included in the modelled process chains. These activities include the **collection, transport and pre-treatment (sorting, separation)** of waste and reusable or recyclable materials (64). Depending on the EoL modelling approach, these activities could be included separately from and unpaired to the core recycling and upgrading treatment (e.g., recycled content approach) (70).

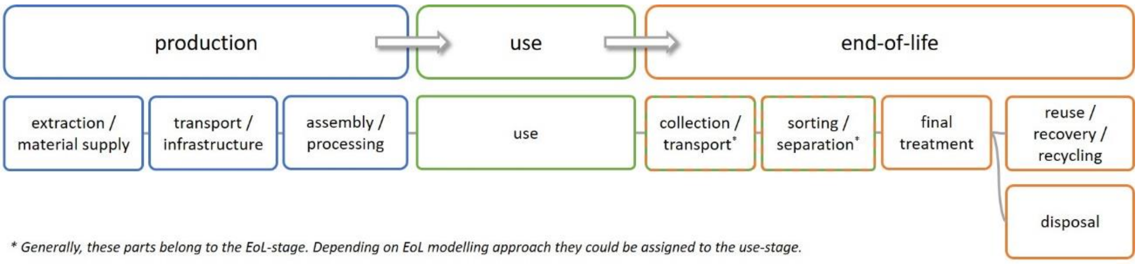


**Figure 8: Simplified structure of a product life cycle with the stages production, use, and end-of-life as well as their sub-stages**

*Waste disposal*

If process flows are classified as **waste**, treatment activities are included and modelled within the system boundaries. Waste treatments describe activities such as **landfilling and incineration** as part of the technosphere (61), whereby **landfill operation and maintenance as well as ash disposal shall be included** (64). Depending on the EoL modelling approach, it is also **possible to consider energy recovery** (and therefore multi-functionality) (64,65), if it is not set to be excluded (71).

*Recycling and reuse*

In the case of further useful materials or components, product systems include **reuse, recovery, and recycling processes**. The implementation can be distinguished by means of the **product system type** and, on the other hand, by the **methodological modelling approach**.

If material flows outside the spectrum of products (e.g. wastes for landfilling or incineration and recyclable material) arise in EoL modelling, these processes can be modelled by **closed- or open-loop schemes** (72). If the material or component keeps a consistent quality and does not change its properties because of the utilisation processes, the procedure applies to **a closed-loop product system** (which corresponds to the substitution approach). Therefore, material and components can be **recirculated back to the same (type of) product system** (1,72). **Open-loop product systems** are associated with diverging **use of the recycled material and components in different product systems** (72). This classification is also linked to a loss of quality and down-cycling (70). A closed-loop procedure also applies to open-loop product systems with consistent product quality and properties (closed-loop approximation) (70,72).

Regarding the **modelling approaches to EoL recycling and reuse** activities, a **wide range of different methods** can be found in the literature (69,72,73). For instance, distinctions are made referring to partitioning by physical relationships, physical properties (mass), or by economic values (14), different underlying system levels (process level, product system level, material life cycle level) (69,74), or weak and strong sustainability concepts (75). Potentially, the application of **different modelling approaches** comes along with **different adjusted system boundary settings** (70). Exemplary approaches and links to further specific solutions for EoL modelling can be found in the box "*EoL modelling methods*".

*Lack of data*

A recurring problem in cases of novel or emerging technologies EoL is the **lack of data on utilisation and disposal options**. This fact also applies to FCH-related EoL technologies and strategies (76). Exemplary ways of dealing with these circumstances vary from omitting the EoL phase (77) to the **consideration of the worst-case scenario** by assuming landfilling (78). The latter approach was previously recommended by previous FCH-specific LCA guidelines (10). It is recommended to apply a **sensitivity analysis for at least one applicable recycling solution** to provide an estimation in the overall context (exemplary options in (76)). Generally, the procedure depends on the applied modelling approach.

**Box 25. Equipment End-of-Life I**

To conduct LCA studies regarding "end-of-life" in line with these guidelines for FCH systems, the following **requirements shall be fulfilled**:

1. The EoL of FCH technologies shall be considered. ●●●●●
2. Preparatory steps (collection, transport, pre-treatment (sorting, separation)) of EoL flows shall be considered, if not excluded by method. ●●●●○
3. Downstream activities of waste treatment, such as landfill operation and maintenance as well as ash disposal, shall be included. ●●●●○
4. The choice of the modelling approach to EoL shall be documented and justified. ●●●●○
5. System boundaries shall be drawn in line with the underlying EoL modelling approach. ●●●●●

**Box 26. Equipment End-of-Life II**

When considering "end-of-life" in LCA studies in line with these guidelines for FCH systems, the **following points are recommended**:

1. Depending on the modelling method, credits may be given for energy and materials recovery. ●●●○○
2. If no data is available for the waste-treatment activities, a sensitivity analysis for at least one applicable recycling solution and/or a worst case of disposal (landfilling or incineration) should be considered. ●●●○○

*Disposal, recycling and reuse paths and technology*

The EoL treatment technologies can be limited in their development and applicability due to different development states of the previous production and use stages. While currently some hydrogen production and use technologies such as PEMWEs/PEMFCs have reached an important technology maturity, others like solid oxide electrolysers/fuel cells (SOEs/SOFCs) are still under significant development (79,80). These conditions may also influence the availability of suitable technical disposal and recycling solutions. Therefore, the **limitation of technology options can limit the data availability** associated with them. The box "*Exemplary EoL treatment options*" provides exemplary information on EoL treatment options focused on FCH technologies.

**EoL modelling methods**

A recommendation for EoL modelling of FCH technologies is implicitly given by ISO standards for LCA (14) and further guidelines. The topic of multi-functionality influences the modelling of the assessed system. According to method-related publications (70,75), the most common approaches are the "recycled content approach" (cut-off approach), which applies to open-loop recycling, and the "avoided burden approach" (end-of-life recycling approach), which applies to closed-loop recycling. A specific case study on the EoL of FCH technology is given by Lotrič et al. (81) by applying the avoided burden approach. In Nordelöf et al. (70) different aspects and potential application errors of these two approaches are discussed. The approaches are also used by further guidelines like PAS 2050 (82) or GHG Protocol (68).

*Recycled content approach (cut-off approach)* (70,73,75)

Applying the cut-off approach induces that the recovery and upgrading of EoL are "cut off", while the collection, transport and pre-treatment are included in the modelling. The approach requires that no credits are given to the system for "secondary raw material" or energy recovery in the downstream. If the input contains secondary/recycled material in the upstream, the material is burdened with impacts from recovery and upgrading. The reasons for applying the approach depend on the goal of the study. The described "simple cut-off" approach has to be differentiated from "cut-off with economic allocation" and "cut-off plus credit" (73). The approach is also called "100/0 method".

*Avoided burden approach (end-of-life recycling approach)* (70,73,75)

In contrast to the first described approach, the end-of-life recycling approach includes the collection, transport and pre-treatment, as well as the recovery and upgrading in the modelling. The recycled/recovered material replaces primary material in the input of the modelled or other systems, so a credit for the studied product as negative impact is given. To avoid double counting of benefits, the input is modelled with 100% primary material. The approach is also called "0/100 method".

*Circular footprint formula (CFF) approach* (64)

With regard to the application of the Product Environmental Footprint (PEF) method, allocation can be solved by applying the so-called circular footprint formula (CFF). The formula combines "material", "energy", and "disposal". A number of parameters describe primary and secondary material use as well as recycling material minus a credit for avoided primary material, energy recovery minus the credit for avoided primary energy, and the disposal of remaining waste. The distribution of impacts and benefits of recycling (material recovery) occurs between the recycled input material user and the manufacturer of the product that was recycled. The formula is applicable for open-loop and closed-loop recycling systems.

*Other approaches*

Further approaches can be distinguished in terms of allocation procedure (e.g., ISO 14067:2018; market price-based allocation) or their national background (e.g., Dutch Handbook on LCA (83) or the French Environmental Footprint Guidance BPX 30-323 (84)), for example. More detailed formulations of approaches in literature are provided by Gaudreault (69), Rehberger and Hiete (72), Ekvall et al. (73) and Allacker et al. (85) in specific contexts.

### Exemplary EoL treatment options

Regarding prominent FCH technologies such as AWEs, PEMWEs, PEMFCs and SOFCs, literature from the project HyTechCycling and others offer information on contained components and available waste management routes for these technologies (76,78,80).

In Valente et al. (76,86) different waste treatment, recycling and reuse paths are illustrated for SOFCs, PEMFCs, PEMWEs and AWEs. The EoL schemes distinguish between BoP (supporting and auxiliary components) and stack (series-connected cells) and show specific utilisation activities (manual disassembly, mechanical sorting, etc.) and output flows for recycling (e.g., iron, gold) and disposal (e.g., mineral wool).

The publications by Stropnik et al. (78) and Lotrič et al. (81) also offer information on FCH system parts, components, and contained materials up to the utilisation and disposal paths. Additional information on materials classification (e.g., hazardous waste) in Lotrič et al. (81) eases the assignment to specific utilisation routes. While the paper by Stropnik et al. (78) is focused on PEMFCs, the paper by Lotrič et al. (81) deals with hydrogen production by PEMWEs and AWEs and hydrogen use in low-temperature PEMFCs.

Figure 9 provides a general overview on the EoL processes of recycling, reuse and disposal for FCH systems. Depending on the FCH system, the routes and their outputs differ.

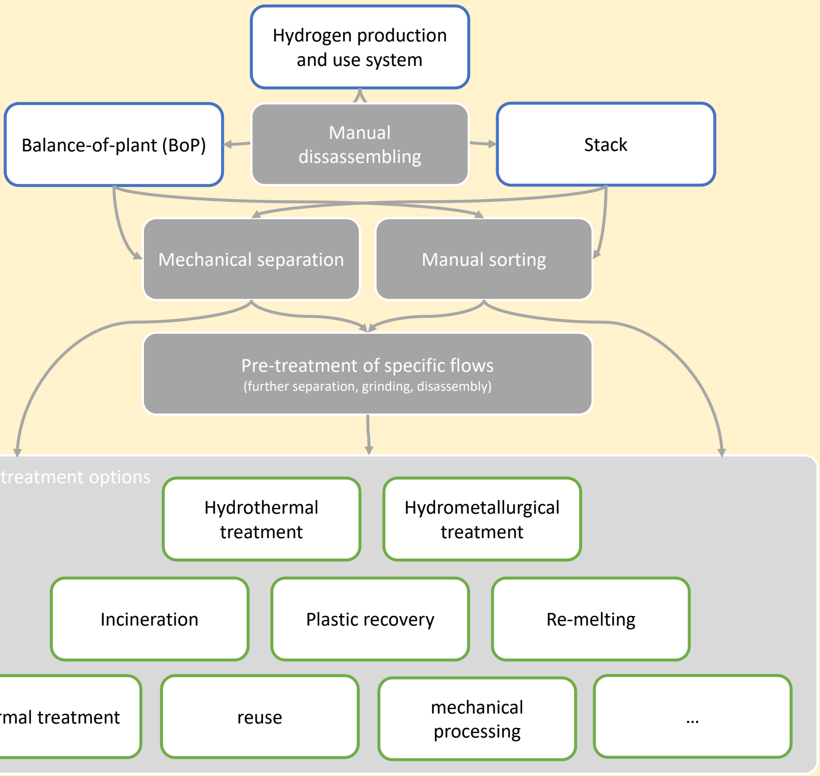


**Figure 9: EoL processes for FCH technologies based on schemes published in** (76)

## 3.4 Multi-functionality

### Motivation

**Multi-functionality** in LCA is observed when a system delivers more than one functional flow (8,87). For many cases, approaches to deal with multi-functionality have been researched over the past years, and reaching a consensus in dealing with multi-functional systems is still a challenge (8). The hierarchy defined by ISO 14044 and 14040 and ILCD prioritises subdivision, system expansion, and, in the last case, the application of allocation (1,14,19). Comparing consequential and attributional LCA, often system expansion is more applied for the first one (8,19). In contrast, for attributional LCA, allocation is often found as an appropriate solution (8,19).

Systems producing and/or using hydrogen often lead to different outputs, and, in many cases, these outputs are considered valuable products, resulting in multi-functional processes. Even though previous FCH-specific LCA guidelines already addressed hydrogen-related multi-functionality cases (10,16), the review performed in the scope of the SH2E project (17) pointed out that the approaches to deal with multi-functionality in many publications and European projects are not totally in agreement with existing guidelines, or, in many cases, the applied strategies are not even mentioned in the publications. Therefore, these guidelines propose a comprehensive approach to deal with multi-functionality for systems producing and/or using hydrogen for energy-related applications. This builds upon the existing generic (1,14,19) and hydrogen-specific (10,16) guidelines.

## Description of the topic

**Hydrogen** can be produced through different pathways, which means that different additional products can be obtained during its production. These products have several properties and applications, indicating the need for distinct approaches to solve the **multi-functionality** of the processes, aligned to the ISO 14040/14044 standards and ILCD (i.e., **subdivision**, **system expansion**, and **allocation**) (1,14,19). Therefore, for systems producing hydrogen and other products, in which hydrogen is the quantitative reference of the modelled process in the LCA, it is to be defined whether hydrogen is the **main product** or a secondary product (**co**- or **by-product**) of the studied process (without considering the LCA perspective). For systems using hydrogen, the guidelines consider if the studied system is a **fuel cell** or another **system using hydrogen** for different applications.

## Options

Different cases can be distinguished for multi-functionality:

- **Case 1**: Systems producing hydrogen.
    - 1a. Hydrogen as the main product.
    - 1b. Hydrogen as a co- or by-product.

- **Case 2**: Systems using hydrogen.
    - 2a. Fuel cells.
    - 2b. Other systems using hydrogen.

## Requirements and recommendations

### General requirements and recommendations

For processes delivering more than one function, it is necessary to identify the most suitable approach to solving the multi-functionality issue. For that reason, the first step is the identification/confirmation if the process can be really considered as a multi-functional process, through the identification of the functional and non-functional flows (Box 27) (8). For instance, if, besides the product flow, all the output flows are elementary flows, then it is not a case of multi-functionality, as elementary flows (resources/emissions from/to nature) are not considered functional flows.

**Box 27. Multifunctionality I**

It must be identified if the studied process is a case of multi-functionality or not through the identification of the functional flow(s).

In case the studied process is identified as a multi-functional process, then the ISO 14040/14044 recommendation shall be applied, according to Box 28 (1,14). Therefore, allocation should be avoided by applying subdivision or system expansion (cf. Key terms), if possible. In case allocation cannot be avoided, then a physical relationship should be preferred for the definition of the allocation factors.

**Box 28. Multi-functionality II**

1. In case of multi-functionality, allocation needs to be avoided by the application of division of unit processes into different sub-processes, according to the outputs produced.
2. Another alternative to avoid allocation is, when appropriate, the application of system expansion.
3. If allocation cannot be avoided, allocation must be applied partitioning inputs/outputs according to the physical relationships between them or other possible relationship (e.g., economic).

### Requirements and recommendations for systems producing and/or using hydrogen

Following the general recommendations, first, it must be identified if the other outputs of the process are, in fact, functional flows (Box 27). In case they can be considered emissions to nature (e.g., in many processes oxygen as an output can be regarded in this way), then elementary flows should be selected, indicating that it is not a case of multi-functionality. If the output can be considered a waste of the process, then a waste flow should be applied, and the waste treatment process should be selected.

However, if the outputs are indeed considered product flows, this indicates that one of the approaches defined by the ISO 14040/14044 hierarchy should be applied (Box 28). The particularities arising from each case (systems producing and using hydrogen and their specific subcases) are detailed in the next paragraphs. Lastly, if it is needed to apply allocation, the mass allocation for systems producing hydrogen should be avoided, and allocation based on energy content should be preferred for cases where hydrogen is applied for energetic purposes and the other products are also energy carriers (88) (Box 29).

**Box 29. Multi-functionality for systems producing and/or using hydrogen I**

In case allocation is applied:

1. Allocation based on the mass must be avoided, as the energy/mass ratio for hydrogen is higher than for other products. Energy-based allocation is preferred (clearly stating the energy basis) when possible.

As in previous FCH-specific LCA guidelines (10,16), it is recommended to explore the effect of the approaches to deal with multi-functionality through sensitivity analysis (Box 30).

**Box 30. Multi-functionality for systems producing and/or using hydrogen II**

Additionally, it should be considered that:

1. Sensitivity analysis is recommended in order to compare the different approaches to deal with multi-functionality and explore the influence of system expansion, allocation, and subdivision (if possible) on the results.

- **Case 1: Systems producing hydrogen**

**Case 1a. Hydrogen as the main product**

Following the general recommendation, the first possibility to solve multi-functionality for systems producing hydrogen is the application of subdivision, which is in many cases not possible, as usually the same processes deliver different products (10,16).

The second step in the hierarchy is the application of system expansion for the other products. To select the alternative system, allowing to account for the credits of system expansion, it must be identified if hydrogen is the main product from an industrial perspective, and if there are other possible processes producing the other outputs. System expansion is not always possible, as sometimes it is challenging to define an alternative process. System expansion is suggested for processes in which hydrogen is the main product, such as water splitting (89). For instance, it is possible to apply system expansion and consider cryogenic distillation or another relevant technology (88) as an alternative for oxygen production, as water splitting usually aims to produce hydrogen and there are other alternatives to produce the oxygen additionally produced. For systems also producing heat and/or electricity, the use of the region's market as an alternative is suggested (88).

**Box 31. Multi-functionality for systems with hydrogen as main product I**

If it is not possible to apply subdivision, system expansion needs to be applied to processes in which hydrogen is the main product (from an industrial perspective, e.g., water splitting - electrolysis).

For system expansion application in water splitting processes, if oxygen is an output and functional flow, then cryogenic distillation or another technology needs to be defined as an alternative for production.

If heat/electricity is produced as an additional product, regional processes related to the production of electricity and/or heat are options to be selected.

Following the ISO standard hierarchy, the next possibility would be the application of allocation. The two main allocation possibilities are economic and physical allocation. When dealing with hydrogen, it must be considered that mass allocation is not recommended (88), as this would associate a low ratio of the impacts to the hydrogen production. Hence, the first recommendation when applying allocation is the use of physical allocation using the energy content (clearly stating the energy basis; e.g., lower heating value), however this is not possible for many secondary products (88). If considering the energy content is not feasible, due to the characteristics of the obtained products, then physical allocation based on number of moles is suggested, if the calculation of the number of moles is possible. Otherwise, prioritising non-physical allocation (e.g. economic allocation) is recommended. Economic allocation is suggested for the cases in which the previous alternatives are not representative of the system and/or where the economic aspects of the products are relevant. The economic values selected should be from the same studied region (88). In addition, the investigation of price oscillations over the past two years should be considered through a sensitivity analysis if relevant. Finally, if economic aspects are not relevant to distinguish the different outputs of the process, then the recommendation is the application of physical allocation based on the mass, as a last possibility. In all cases, sensitivity analyses are recommended to investigate and compare the different approaches to deal with multi-functionality.

### Box 32. Multi-functionality for systems with hydrogen as main product II

If it is not possible to apply system expansion, physical allocation based on energy content needs to be applied when only energy-carrier products are involved. If not possible, physical allocation based on number of moles must be selected, otherwise economic allocation is suggested. If there is no economic relevance or the previous alternatives are not possible, mass allocation should be applied as a last option, and the limitations of this application should be stated.

### Box 33. Multi-functionality for systems with hydrogen as the main product III

For economic allocation, the selected economic values should be for the same region under study. If economic allocation is applied, sensitivity analysis should be applied investigating economic value oscillation over two years (if relevant).

### Case 1b. Hydrogen as a co- or by-product

For systems producing hydrogen as a co- or by-product, application of subdivision is expected to be challenging since, usually, the same process delivers different products.

The second step in the hierarchy is the application of system expansion. In processes as chlor-alkali electrolysis (where the products are hydrogen, chlorine, and sodium hydroxide), it might not be possible to select the alternative process for the chlorine and sodium hydroxide production (16,90). The same applies to steam cracking, as it would be challenging to define alternative processes for the production of olefins (9). In this way, system expansion may not be possible for systems producing hydrogen in which hydrogen is considered the by-product of the process from an industrial perspective, even if for the performed LCA hydrogen is considered the quantitative reference.

Following the ISO standard hierarchy, the next possibility would be the application of allocation. For this case, the same conditions presented in case 1a (hydrogen as the main product) can also be applied. The approach to model processes producing hydrogen when multifunctionality occurs can be summarised according to Figure 10.

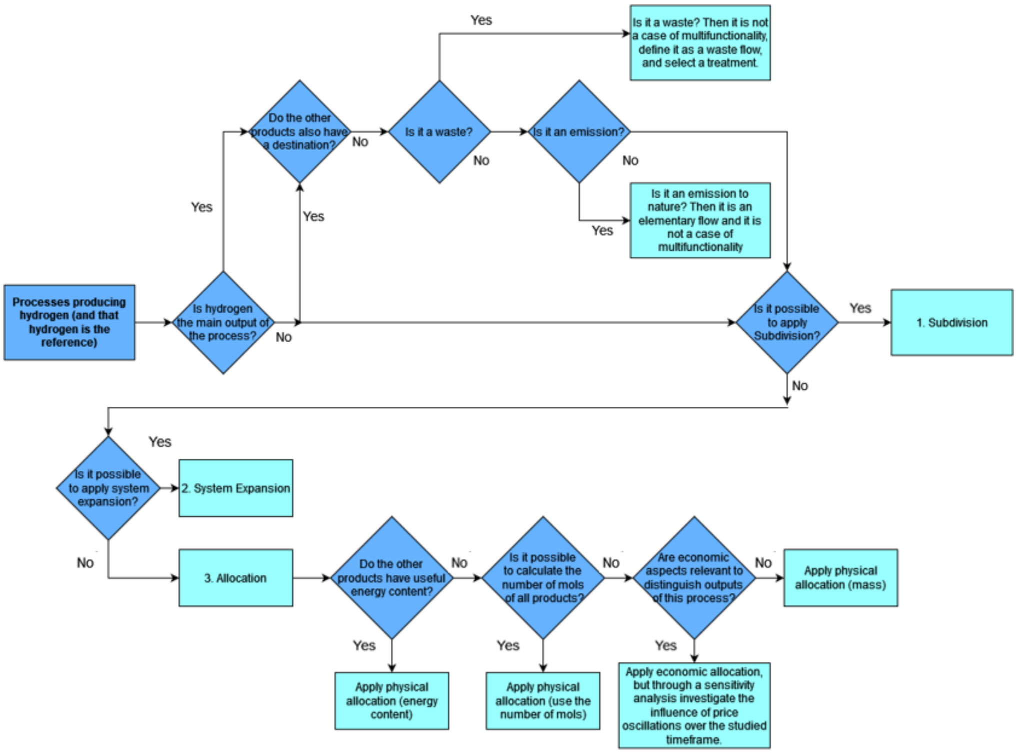


Figure 10. Decision diagram

- **Case 2: Systems using hydrogen**

### Case 2a. Fuel cells

One of the most common hydrogen applications in fuel cells is to generate electricity and heat, which can be considered both valuable products in many cases. Therefore, this would represent a case of multi-functionality. The produced water is usually not a functional flow, as it can be modelled as a waste. For this case, it might be not possible to apply subdivision, as the same system is generating both products. On the other hand, sometimes system expansion can also constitute an issue in case it is needed to identify a representative alternative for heat production. Lastly, if allocation needs to be applied, then relationships for the allocation factors should be defined (10).

When heat is considered as a valuable product, then approaches to solving the multi-functionality should be defined. According to previous FCH-specific LCA guidelines (10), one possibility is the calculation of exergy in order to allocate the impacts between the heat and the electricity. Otherwise the heat should be modelled as an emission to the environment (therefore an elementary flow, and not a case of multi-functionality), and the water produced in fuel cells can also be modelled as an elementary flow (8,10).

Hence, following the approach defined in the previous cases, the first step also for solving multi-functionality in fuel cells should be the identification of the possible functional flows of the process, in order to confirm if the process actually represents a case of multi-functionality (Box 27). If it is still a case of multi-functionality (confirming that heat is a valuable product), then subdivision should be applied (if possible), otherwise system expansion should be preferred instead of allocation (Box 28). Regarding the application of allocation, exergy should be defined as the functional unit and the reference for allocation (Box 34) (10). If it is not possible to apply physical allocation based on the exergy, then economic allocation should be applied (Box 34). Finally, the different approaches to deal with multi-functionality should be investigated through sensitivity analysis (Box 30) and sensitivity analysis to investigate the effects of economic values oscillation is also recommended for economic allocation (Box 33).

### Box 34. Multi-functionality in fuel cells

For fuel cells constituting a case of multi-functionality, in case physical allocation is applied, exergy must be applied for the calculation of the partitioning factors between electricity and heat. If it is not possible to apply physical allocation, economic allocation is the second alternative for the definition of the allocation factors.

**Case 2b. Other systems using hydrogen**

There is a huge variety of systems that can apply hydrogen for the most distinct functions, therefore for these systems, the approaches to be followed in each case are not specified in the current guidelines. For these cases, the general recommendations for multi-functionality should be respected, and sensitivity analysis to investigate the different approaches and compare their effect in the results is recommended (Boxes 27, 28, 29, 30, and 33).

**Evaluation: "method readiness level"**

- Identification of multi-functionality ●●●●●
- Dealing with multi-functionality in systems producing hydrogen ●●●●○
- Dealing with multi-functionality in systems using hydrogen ●●●○○

**This section is linked to the following section of the present guidelines:**

- 3.2: Scope of the Life Cycle Assessment – Functional Unit
- 3.3: Scope of the Life cycle Assessment – System boundaries
- 3.5: Scope of the Life cycle Assessment – Biogenic carbon emissions and carbon storage

## 3.5 Biogenic carbon emissions and carbon storage

### Motivation

**Carbon capture and storage (CCS)** as well as **carbon capture and utilisation (CCU)** are regarded as technologies that can contribute to decarbonisation and mitigation of emissions from heavily-polluting industries, such as chemical, steel and cement ones (5,6) in the EU. The potential benefits of these technologies for systems producing or using hydrogen are currently under investigation and have been discussed in a number of studies (6,91–93). Furthermore, the production of hydrogen from renewable feedstocks, such as biomass and waste, is seen as an alternative to electrolysis with electricity from renewable sources (93) and an opportunity for sustainable energy (91,94). Modelling decisions regarding CCS and CCU as well as **biogenic carbon** in systems producing and using hydrogen need to be taken, considering **implications on system boundaries and life-cycle impacts**.

### Description of the topic

If carbon capture technologies are installed at a plant, this will benefit from the avoidance or reduction of direct emissions. However, some effort (e.g., energy) will be needed for capturing, transporting and eventually storing $CO_2$. In addition, if captured carbon is further used in subsequent life cycles (e.g., for chemical or energy carrier production), this can be seen as a valuable product feeding other processes. **Questions arise on how to allocate burdens of CCS and CCU** between the different sub-systems, products and co-products involved in FCH systems. Furthermore, if hydrogen is produced from renewable feedstock such as biomass, the practitioner faces choices regarding **modelling of biogenic carbon balance** (biogenic carbon uptake and release) **and credits for biogenic carbon storage**.

## Options

Different cases can be distinguished for carbon modelling of systems producing and/or using hydrogen, considering the presence of CCS or CCU or the inclusion of biomass as raw material for hydrogen production. Specifically:

- **Case 1**: Systems producing hydrogen from fossil sources:
    - 1a. with CCS;
    - 1b. with CCU.
- **Case 2**: Systems using hydrogen and carbon dioxide from CCU technologies for the production of value-added products, such as chemicals and/or energy carriers:
    - 2a. $H_2$ and $CO_2$ produced from two different systems;
    - 2b. $H_2$ and $CO_2$ produced from the same system.
- **Case 3**: Systems producing hydrogen from biomass sources:
    - 3a. without CCS or CCU;
    - 3b. with CCS or CCU.

## Requirements and recommendations

### General requirements and recommendations

As for production plants where **CCS and CCU technologies** are installed, it is important to distinguish between when 1) carbon capture is installed to make the plant cleaner, as in the case of CCS ($CO_2$ is seen here as a waste); and 2) carbon capture is installed to obtain $CO_2$ as a feedstock for a carbon utilisation plant, as in the case of CCU ($CO_2$ is seen here as a valuable co-product). Furthermore**, it should be considered if $CO_2$ needs to be separated from the main product** to make the latter available on the market (as for the production of ethylene oxide (95) and ammonia (96)) and if there are **market changes** in specific $CO_2$ demand (5), in the event that this is considered more and more as a valuable feedstock.

**Box 35. Carbon modelling for CCS and CCU technologies I**

1. If CCS technologies are installed at a production site, the **effort for capturing and storing $CO_2$ must be modelled and attributed to the produced main product**. It is assumed that CCS is implemented with the purpose of reducing plant pollution.
2. If CCU technologies are installed at a production site (first system), the **effort for capturing and utilising $CO_2$ must be attributed to the plant** (second system) **using the carbon as feedstock**. It is assumed that capturing and preparing the feedstock for further application is responsibility of the second system.

Deviation from the proposed CCU and CCS modelling shall be explained and justified by the practitioner.

### Box 36. Carbon modelling for CCS and CCU technologies II

Additionally, it should be considered that:

1. Recommendations for CCU burden attribution may change **if further effort is required for the separation of $CO_2$ from the main product** produced by the first system. In this case, the effort for capturing and using $CO_2$ should be split between the first ($CO_2$ emitter) and second ($CO_2$ user) systems. Assuming that the carbon capture is needed by the first system to have a marketable product and by the second system as input material for subsequent $CO_2$-based products, it is proposed to **apply a 50:50 allocation** between the two systems for the $CO_2$ capture and separation burdens.
2. Recommendations for CCU and CCS burden attribution may change **if $CO_2$ becomes scarce in the market** and, therefore, this is regarded as a co-product with market value. In this case, other allocation rules can be followed, such as 50:50 or 0:100 split of the burdens between the first ($CO_2$ emitter) and second ($CO_2$ user) system.

As for plants producing **$CO_2$-based products**, it appears important to consider the interaction between the $CO_2$ primary emitter plant and the CCU technology; the first (primary emitter and $CO_2$ source) and second (CCU and $CO_2$ user) systems are linked and depend on each other, and it appears difficult to separate them in the boundaries of the study. In some cases, the primary emitter and the CCU plant operate independently. However, the primary emitter plant can experience some changes in the production output if the CCU plant is installed (5), for instance if some energy produced by the primary emitter is used for carbon capturing and therefore less of the main product of the first system is produced in comparison to when CCU was not installed.

In some cases, the practitioner may want to **compare the environmental impacts of $CO_2$-based products**, for instance synthetic fuels, where $CO_2$ has different origin depending on the primary emitter. Including the primary emitter in this comparison is not applicable if the function of the compared systems is not the same: it is not feasible to compare e.g. system A, which has the function to produce main product A (e.g. electricity) and the $CO_2$-based product (synthetic fuel C), and system B, which has the function to produce main product B (e.g. cement) and the $CO_2$-based product (synthetic fuel C). To enable such comparison, only the function of producing the $CO_2$-based product needs to be studied: to exclude the function of producing the main product, the attribution of burdens of the primary emitter between the main product and the $CO_2$ for the CCU plant becomes a case of multi-functionality.

### Box 37. Carbon modelling for CCS and CCU technologies III

1. When $CO_2$-based products are modelled, **the boundaries of the study should include the $CO_2$ source, the CCU technology and the $CO_2$-based product**. 100% of $CO_2$ emitter burdens should be attributed to the main product produced by the first system, while effort for CCU should be attributed to the $CO_2$-based product (5).
2. When the goal of the study is to **compare $CO_2$-based products and the function of the compared systems is not the same**, only the function of producing the $CO_2$-based product should be included in the functional unit and system boundary definition. Therefore, the attribution of primary emitter burdens between the main product of the $CO_2$ primary emitter plant and the $CO_2$ should be managed as a case of multi-functionality, hence following the general recommendations reported in the dedicated Section 3.4. Burdens for capturing the $CO_2$ should be attributed to the $CO_2$-based product.

Additional recommendations from Box 36 also apply here. Deviation from the proposed system boundaries shall be explained and justified by the practitioner.

### Box 38. Carbon modelling for CCS and CCU technologies IV

Additionally, it should be considered that:

1. If the primary emitter changes its operation due to the installation of CCU technologies, **compensation of these changes** should be attributed to the second system (CCU) (5). For instance, if some energy (heat or electricity) produced by the first emitter is used to power the carbon capturing process, the first system (primary emitter and $CO_2$ source) will not be able to achieve the same energy output as before without CCU. Therefore, the production of additional energy, e.g. from external sources, needs to be considered to fulfil the same functional unit of the system as without CCU. The effort for producing this additional energy to compensate production changes in the first system when the CCU is implemented should be allocated to the second system (the CCU plant).

As for systems using **biomass sources** as input into production processes, attention needs to be paid to the identification of cases of permanent biogenic carbon storage and to accounting of **biogenic carbon balance** (biogenic carbon emissions and release). Furthermore, the **origin of biomass** can be important for allocation decisions, for instance if the organic content is derived from processes with the primary aim of delivering products for the food sector or if biomass is obtained from energy crops (92).

### Box 39. Carbon modelling for CCS and CCU technologies V

1. **Product Environmental Footprint Category Rules** (v.6.3) should be followed for biogenic carbon modelling (2):
    - ○ characterisation factors for biogenic carbon dioxide ($CO_2$) uptake and emissions are zero;
    - ○ **carbon credits are attributed only for cradle-to-grave** studies when **biogenic carbon storage time >100 years**, or if biogenic carbon storage in forest + lifetime of final product >100 years;
    - ○ no carbon credits are attributed for a cradle-to-gate study.

Deviation from the proposed rules shall be explained and justified by the practitioner.

### Box 40. Carbon modelling for CCS and CCU technologies VI

Additionally, it should be considered that:

1. If biomass has not been produced for the purpose of being a feedstock for a production process, 100% biomass production burdens can be allocated to the previous life and not to the system using it (**cut-off approach**).
2. Please refer to Sections 3.3 and 3.4 about system boundaries and multi-functionality for general recommendations on how to deal with multi-output processes concerning biomass production.

### Requirements and recommendations for systems producing and/or using hydrogen

Recommendations for hydrogen systems build on the previous general requirements and recommendations for carbon modelling.

- **Case 1**: Systems producing hydrogen from fossil sources

**Case 1a. with CCS**: it is assumed that $CO_2$ would be produced anyway besides $H_2$ (97), the main product for which the production process is established. Please consider that this may change if the market requests more and more $CO_2$ and specific production pathways for $CO_2$ are defined (98). In the current situation, carbon capture and storage is installed to make the system cleaner and reduce or avoid carbon emissions.
**Recommendation**: attribute 100% of system burdens to $H_2$, including effort for CCS (91,92,99), as outlined in Box 35 and Figure 11 for the proposed system boundaries.

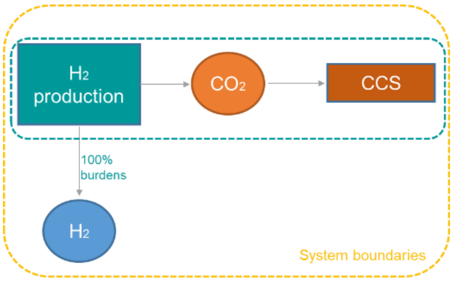


Figure 11: Recommended system boundaries of Case 1a: Systems producing $H_2$ from fossil sources with CCS

**Case 1b. with CCU**: $CO_2$ is considered as a feedstock for a CCU plant (5); it is assumed that it is not responsibility of the $H_2$ production system to treat and make $CO_2$ in a status usable by the second system, therefore the preparation of the product is related to the $CO_2$ further value chain. Furthermore, the CCU plant makes it possible that less or no $CO_2$ is emitted to the environment by the hydrogen production process (5). **Recommendation**: attribute 100% of the system burdens to $H_2$ excluding effort for CCU, as outlined in Box 35 and Figure 12 for the proposed system boundaries. Note that this does not apply if $CO_2$ needs to be separated from $H_2$ to make the latter available on the market (in this case please refer to Box 36, point 1).

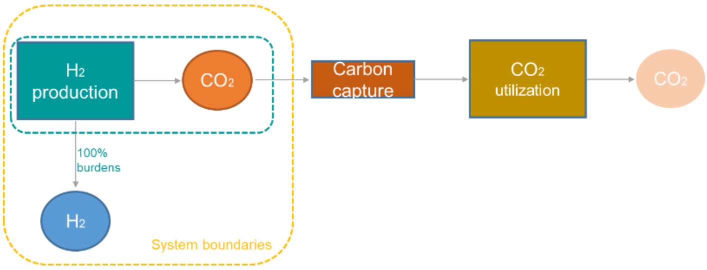


**Figure 12: Recommended system boundaries of Case 1b: Systems producing $H_2$ from fossil sources with CCU**

- **Case 2**: Systems using hydrogen and carbon dioxide from CCU technologies for the production of value-added products, such as chemicals and/or energy carriers

**Case 2a. $H_2$ and $CO_2$ produced from two different systems**: the life cycle of the primary emitter is linked to and dependent on the one of the $CO_2$-based products. The $CO_2$ from the primary emitter and the $H_2$ from another production process are both valuable inputs into the $CO_2$ utilisation. **Recommendation**: include the $CO_2$ source, CCU, $CO_2$-based product, $H_2$ production in the system boundaries. As for the sub-systems, attribute 100% of primary emitter burdens to the main product A from the primary emitter and attribute effort for carbon capture to $CO_2$-based product. Please refer to Box 37, Box 38 and Figure 13 for the proposed system boundaries.

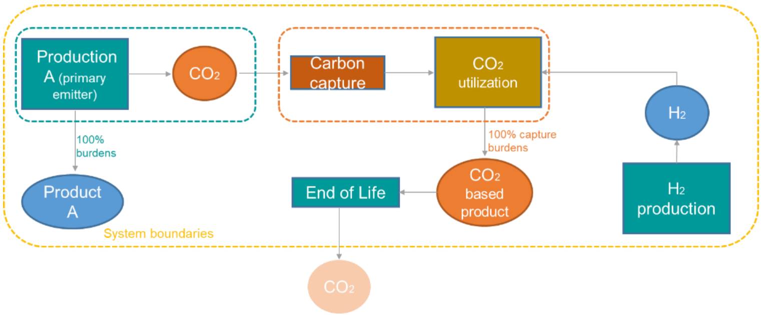


**Figure 13: Recommended system boundaries of Case 2a: Systems using $H_2$ and $CO_2$ from CCU technologies ($H_2$ and $CO_2$ produced from two different systems)**

**Case 2b. $H_2$ and $CO_2$ produced from the same system:** in this case, the primary emitter is a process producing both $H_2$ and $CO_2$. These are both used as input for the production of a $CO_2$-based product. However, it can occur that not all captured $CO_2$ is needed as feedstock for the subsequent process and that a share is therefore used outside the system boundaries. **Recommendation**: include the $CO_2$ source ($H_2$ production), carbon capture, carbon utilization effort (as for the $CO_2$ share needed for the $CO_2$-based product) and the $CO_2$-based product itself in the system boundaries. Please consider Box 37, Box 38 and Figure 14 for the proposed system boundaries. Please refer to Section 3.4 (case 1a "hydrogen as the main product") for recommendations on how to split burdens of the primary emitter between $H_2$ and $CO_2$.

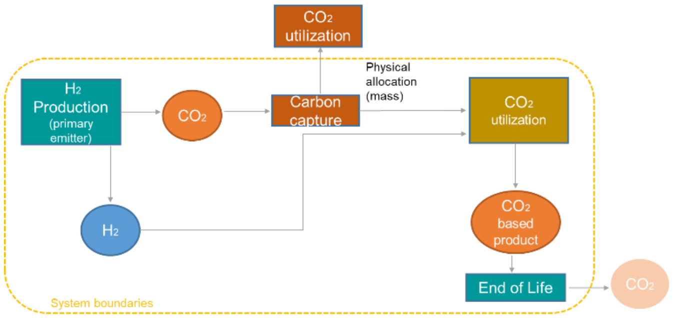


**Figure 14: Recommended system boundaries of Case 2b: Systems using $H_2$ and $CO_2$ from CCU technologies ($H_2$ and $CO_2$ produced from the same system)**

- **Case 3**: Systems producing hydrogen from biomass sources

**Case 3a. without CCS or CCU**: depending on the biomass source, $CO_2$ can be sequestered for a certain amount of time (e.g., in wood). A cradle-to-grave approach allows to describe the balance between biogenic carbon uptake and releases as well as the benefits of biogenic carbon storage. **Recommendations**: follow PEFCR (2) for carbon balance modelling (characterisation factors for biogenic $CO_2$ uptake and release set to zero) and carbon credits (only for cradle-to-grave studies if biogenic carbon storage can be considered permanent, i.e. > 100 years). Please consider Box 39 and Figure 15 for the proposed system boundaries. Furthermore, as explained in Box 40 and shown in Figure 16, in some cases it can be decided to exclude the biomass source from the system boundaries following a cut-off approach, for instance because biomass was produced for the food sector rather than as an energy feedstock (thus considered a waste for hydrogen applications) or because a gate-to-gate approach was applied (92,94,99). Also in this case, it is recommended to apply the PEFCR guidelines for biogenic carbon modelling and assessment. Specifically, no credits for biogenic carbon storage shall be assigned in this case, as the study is not cradle-to-grave.

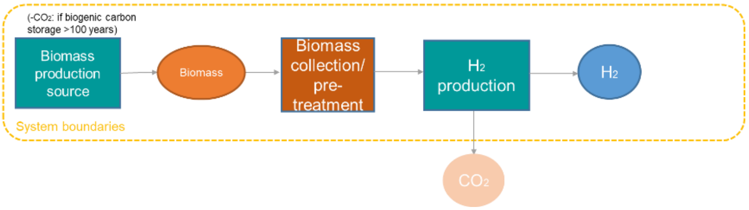


**Figure 15: Recommended system boundaries of Case 3a: Systems producing $H_2$ from biomass sources without CCS or CCU**

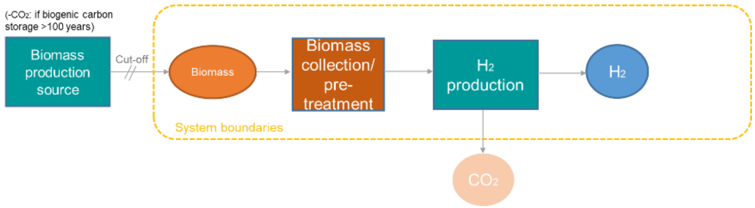


**Figure 16: Alternative system boundaries of Case 3a: Systems producing $H_2$ from biomass sources without CCS or CCU (biomass source cut-off from the system boundaries)**

**Case 3b. with CCS or CCU**: this sub-case can be seen as a combination of the previous Case 3a modified with Case 1a (for CCS) or 1b (for CCU). Therefore, instructions in Box 35 and Box 36 can be combined with those in Box 39 and Box 40, and system boundaries from Figure 11 or Figure 12 can be combined with Figure 15 or Figure 16.

**Evaluation: “method readiness level”**

- CCS modelling ●●●○○

- CCU modelling ●●●○○
- Biogenic carbon modelling ●●●●○

**This section is linked to the following section of the present guidelines:**

- 3.1: Scope of the Life Cycle Assessment – Modelling approach
- 3.2: Scope of the Life Cycle Assessment – Functional Unit
- 3.3: Scope of the Life cycle Assessment – System boundaries
- 3.4: Scope of the Life Cycle Assessment – Multi-functionality
- 5: Life Cycle Impact Assessment

# 4. Life Cycle Inventory

## 4.1 Data sources and availability

### Motivation

LCA models use data for assessing the life cycle of their 'object of study'. Data collection is often seen as a bottleneck in LCA (100). Collected data have a direct influence on model results and insights. Nowadays, it is common to draw on generic databases for completing data needed in an LCA model, especially for those (background) parts that are not specific to the object of study (which is often the case for transport, electricity, infrastructure, input chemicals, etc.). In many studies, generic data contributes to more than 90% of the life-cycle impacts.

Available data and data sources are thus an important LCA topic. For newly collected data, there is the question of how data can be collected, and how data from various primary sources can be brought together and aligned in one LCA model. For generic data sources, there is the question about the best-suited source(s) for data required by the LCA model. And for all data together, alignment and consistency are important both across the data in the LCA model and also with respect to the goal and scope of the LCA model and study.

While these statements apply to any LCA model, the assessment of FCH systems is expected to usually require more diverse data, for example for setting up learning curves and prospective models, and for modelling the risk in the life cycle.

### Requirements and recommendations

Data sources and data availability have a strong link to the goal and scope of the LCA, as well as to quality assurance, data quality, and verification. Only recognised, specific and consistent sources for secondary data are permitted.

Besides, the different steps for the production of LCA data and LCA models could be seen as a "supply chain" as follows:

- it starts from raw data;
- these raw data are potentially reviewed;
- it is brought into a unit process, typically combining different data sources, via reviewed and/or transparent procedures;
- resultant "method-agnostic" datasets are designed to allow flexible adaptation to different modelling needs and methods and can be reviewed;
- then, datasets are made method-specific (goal and scope; multi-functionality, reference data, possible extensions such as risk or scale-up), ideally through a transparent and reviewed procedure;
- if needed, as a next step, datasets are aggregated, e.g. via scripts that are reviewed and open source;

- as a final step in the application of the datasets, an LCA model (and case study) is set up, where the different data are connected, following goal and scope; this connection should ideally be done in a transparent way and reviewed.

In this way, the whole system can create a flexible data structure on demand. Already developed elements can be reused for future studies. The evaluation schema needs to be developed in order to be able to understand best available datasets (Box 41) beyond the dataset “direct” data quality.

Data source maintenance and governance are not considered in the assessment so far. The evaluation focuses on transparency and credibility of the information provided, which is enhanced by a review performed. It should be noted that data quality is considered in a separate section (Section 4.2).

### Box 41. Data sources traceability

Every data source has to be clearly stated (thus ensuring data traceability), and an assessment of transparency and credibility is recommended (cf. Box 42).

### Box 42. Evaluation of data transparency

For LCA data sources, it is proposed that the evaluation follows this table:

| # | step | evaluation | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | raw data reviewed? | reviewed | 5 | not reviewed | 1 | | | | |
| 2 | unit process creation via transparent procedures that are reviewed? | reviewed and transparent | 5 | transparent | 4 | reviewed | 3 | not reviewed not transparent or unknown | 1 |
| 3 | method-agnostic datasets reviewed? | reviewed | 5 | not reviewed | 1 | | | | |
| 4 | method-specific dataset creation via transparent procedures that are reviewed? | reviewed and transparent | 5 | transparent | 4 | reviewed | 3 | not reviewed not transparent or unknown | 1 |
| 5 | dataset aggregation via transparent procedures that are reviewed? | reviewed and transparent | 5 | transparent | 4 | reviewed | 3 | not reviewed not transparent or unknown | 1 |
| 6 | dataset connection via transparent procedures that are reviewed? | reviewed and transparent | 5 | transparent | 4 | reviewed | 3 | not reviewed not transparent or unknown | 1 |

An aggregation is to be performed following the following formula:

$$s_{tot} = \sqrt[n]{\prod_{i} s_i}$$

With $s_{tot}$ = score total;
$s_i$ = individual score for each of the $n$ steps

With this formula, $s_{tot}$ has a minimum value of 1 and a maximum value of 5. The product reflects that all steps are connected and building on each other. In case one step provides a mix of different scores (e.g., Step 1 with some raw data reviewed and some sources not reviewed), the share of the different evaluation scores is used (e.g., if 50% of the sources are reviewed and 50% are not reviewed, the overall score in Step 1 would be 0.5*1 + 0.5*5 = 3).

**Evaluation: “method readiness level”**

- Assessment of credibility and transparency in LCA data sources ●●○○○

**This section is linked to the following sections of the present guidelines:**

- 2: Goal of the Life Cycle Assessment
- 4.2: Life Cycle Inventory – Data quality
- 6.2: Interpretation and final remarks – Verification and validation

## 4.2 Data quality

### Motivation

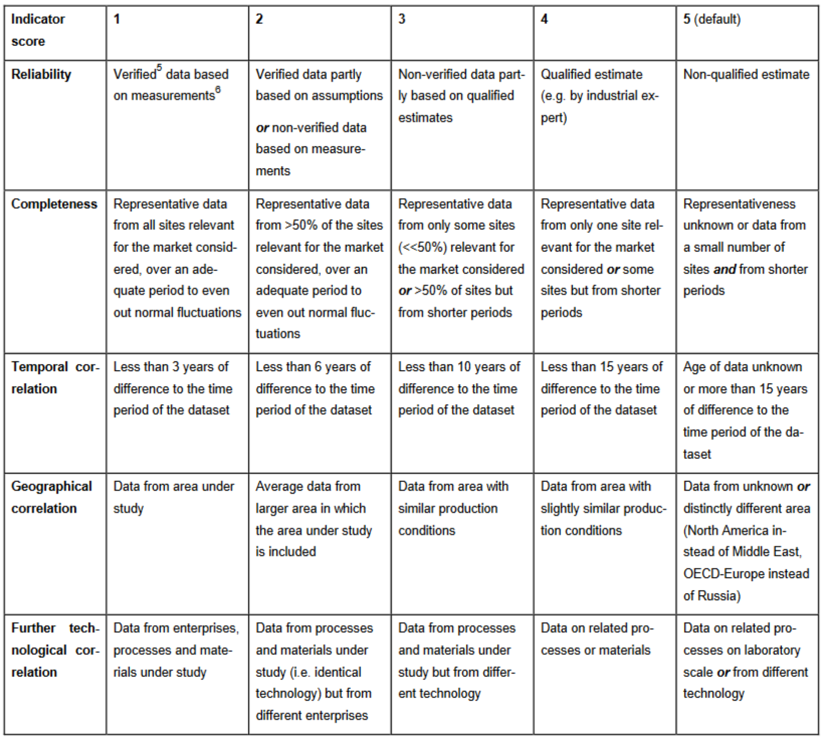
LCA is generally seen as a methodology for decision support. For any decision, the reliability of the information considered, and to question how far the considered information fits the decision at stake, is crucial. Data quality addresses how well information fits the stated requirements, and thus, for example, a decision.

### Description of the topic

Data quality is defined in ISO 14040/14044 as fitness for purpose (1). According to the definition, data quality is not a final, given attribute of stored data, but it rather results from a comparison of given data attributes to requirements. These requirements may be implicitly or explicitly stated, e.g. in goal and scope of an LCA, or come out of a decision situation. If the requirement is to obtain a dataset from 2019, a dataset from 2022 is good but not perfect; if the goal is to obtain a dataset from 2022, a dataset from 2022 fits perfectly.

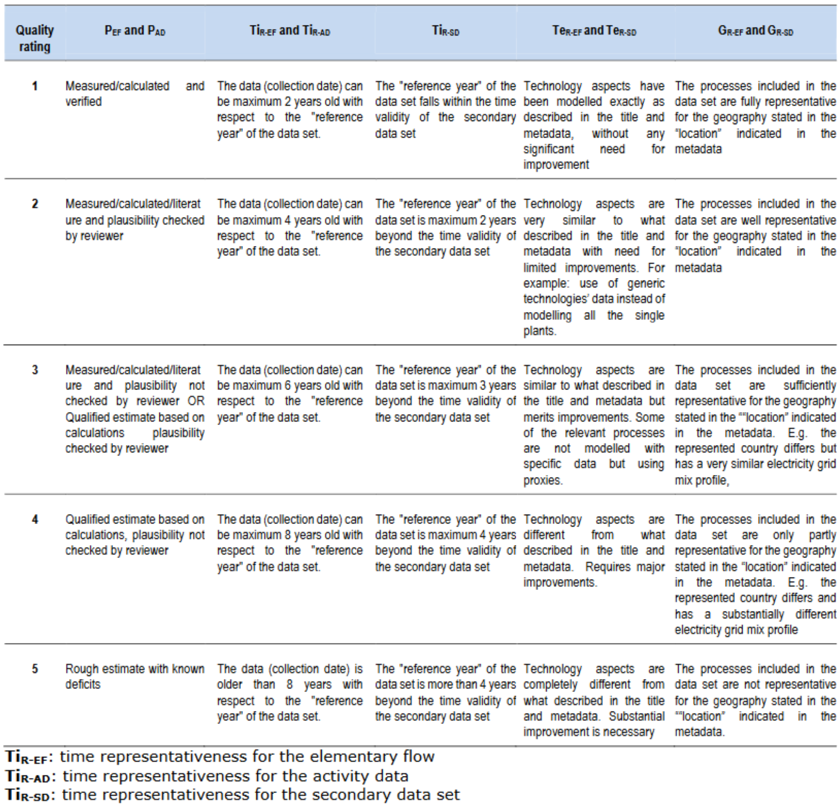
There are typically several facets or aspects of data quality and thus, there are several indicators for data quality considered. Data quality has a long history also in LCA, with SETAC working groups in the 1990’s (101). As per today, there are data quality systems in place and proposed by major LCA databases and by major political actors dealing with LCA. An overview can be found in (8).

Since some time, a “pedigree” approach is common for data quality systems. A pedigree matrix approach basically sets up a table with the different selected data quality indicators, and then assigns scales from 1 to e.g. 5 per indicator, depending on qualitative state descriptions and evaluations. A prominent example is the pedigree matrix used in the ecoinvent database (Figure 17); a slightly different version is also used in the Environmental Footprint (EF) methodology (Figure 18). Both tables are similar. Sometimes, the ratings use very similar text but gives different scores (less than 6 years between time in the dataset and goal is 2 in ecoinvent and 3 in EF). EF does not have the completeness indicator in ecoinvent; EF distinguishes time for data collection and the reference year of the dataset.



| **Indicator score** | **1** | **2** | **3** | **4** | 5 (default) |
|---|---|---|---|---|---|
| **Reliability** | Verified[5] data based on measurements[6] | Verified data partly based on assumptions<br>***or*** non-verified data based on measurements | Non-verified data partly based on qualified estimates | Qualified estimate (e.g. by industrial expert) | Non-qualified estimate |
| **Completeness** | Representative data from all sites relevant for the market considered, over an adequate period to even out normal fluctuations | Representative data from >50% of the sites relevant for the market considered, over an adequate period to even out normal fluctuations | Representative data from only some sites (<<50%) relevant for the market considered ***or*** >50% of sites but from shorter periods | Representative data from only one site relevant for the market considered ***or*** some sites but from shorter periods | Representativeness unknown or data from a small number of sites ***and*** from shorter periods |
| **Temporal correlation** | Less than 3 years of difference to the time period of the dataset | Less than 6 years of difference to the time period of the dataset | Less than 10 years of difference to the time period of the dataset | Less than 15 years of difference to the time period of the dataset | Age of data unknown or more than 15 years of difference to the time period of the dataset |
| **Geographical correlation** | Data from area under study | Average data from larger area in which the area under study is included | Data from area with similar production conditions | Data from area with slightly similar production conditions | Data from unknown ***or*** distinctly different area (North America instead of Middle East, OECD-Europe instead of Russia) |
| **Further technological correlation** | Data from enterprises, processes and materials under study | Data from processes and materials under study (i.e. identical technology) but from different enterprises | Data from processes and materials under study but from different technology | Data on related processes or materials | Data on related processes on laboratory scale ***or*** from different technology |

**Figure 17: Pedigree table for data quality assessment in ecoinvent 3** (102)



| **Quality rating** | **$P_{EF}$ 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 data set. | The "reference year" of the data set falls within the time validity of the secondary data set | Technology aspects have been modelled exactly as described in the title and metadata, without any significant need for improvement | The processes included in the data set are fully representative for the geography stated in the "location" indicated in the metadata |
| **2** | Measured/calculated/literature and plausibility checked by reviewer | The data (collection date) can be maximum 4 years old with respect to the "reference year" of the data set. | The "reference year" of the data set is maximum 2 years beyond the time validity of the secondary data set | 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 modelling all the single plants. | The processes included in the data set are well representative for the geography stated in the "location" indicated in the metadata |
| **3** | Measured/calculated/literature and plausibility not checked by reviewer OR Qualified estimate based on calculations plausibility checked by reviewer | The data (collection date) can be maximum 6 years old with respect to the "reference year" of the data set. | The "reference year" of the data set is maximum 3 years beyond the time validity of the secondary data set | Technology aspects are similar to what described in the title and metadata but merits improvements. Some of the relevant processes are not modelled with specific data but using proxies. | The processes included in the data set 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, |
| **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 data set. | The "reference year" of the data set is maximum 4 years beyond the time validity of the secondary data set | Technology aspects are different from what described in the title and metadata. Requires major improvements. | The processes included in the data set 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 data set. | The "reference year" of the data set is more than 4 years beyond the time validity of the secondary data set | Technology aspects are completely different from what described in the title and metadata. Substantial improvement is necessary | The processes included in the data set are not representative for the geography stated in the ""location" indicated in the metadata. |

**$Ti_{R\text{-}EF}$**: time representativeness for the elementary flow
**$Ti_{R\text{-}AD}$**: time representativeness for the activity data
**$Ti_{R\text{-}SD}$**: time representativeness for the secondary data set

**Figure 18: Pedigree table for data quality assessment in EF** (103)**, P: precision, Ti: time, Te: technology, Gr: geography**

**Data quality in LCA is often stated for the following "scopes":**

- **for unit process LCA datasets (1a),**
- **for process LCA datasets exchanges (i.e. input/output flows, 1b),**
- **for aggregated datasets sometimes (2),**
- **and for LCA study calculation results (3).**

For aggregated datasets and for calculation results, this requires a decision about how to aggregate data quality scores (104).

In LCA studies, users can set the requirements for the LCA at the goal and scope stage. Taking the definition of data quality as the ability to satisfy requirements, a logical consequence is that users can also set how data quality and its assessment is understood, following these requirements, for the given study. This was emphasised in the UN GLAD working group on data quality (105).

Overall, data quality indicators can be classified as follows:

1. Data quality indicators about **generic LCA "measurement"** (precision, completeness, reliability of the source; time; geography; technology of the modelled "twin" fitting to the object at stake, i.e. the process that is to be modelled); these are reflected in the pedigree tables of EF and ecoinvent for example.
2. Data quality indicators addressing **modelling options** (type of allocation performed; handling of recyclates and other connected life cycles).
3. Data quality indicators about **support** for various inventory or LCIA methods (biogenic carbon modelling, water flow modelling, support for a given LCIA method).

Based on this rather comprehensive classification, the UN GLAD data working group developed about 25 different indicators (8).

A further distinction can be made regarding **how the data quality indicators are assessed**. Often, assessment is performed via expert judgement, which can lead to unsubstantiated claims, and/or it is not explained how values for the indicators are to be obtained. The UN GLAD system foresees a *measurement* for representativeness as one option, and also an explicit distinction whether the assessment is provided by expert judgement or by science-based measurement (8).

A topic sometimes mentioned in the context of data quality assessment is **mutual acknowledgement** (e.g., potential use of datasets already assessed in UN GLAD directly in the context of EF without a new data quality assessment). While this recognition reduces effort, the vague assessment of data quality without specific rules apart from expert judgement makes an acknowledgement difficult.

The **principal structure of a data quality indicator** involves a descriptor, a given goal (the ideal indicator value), a representation (how the indicator is, in the assessed data) and a conformance, as difference between the ideal goal and the representation (Figure 19) (106).

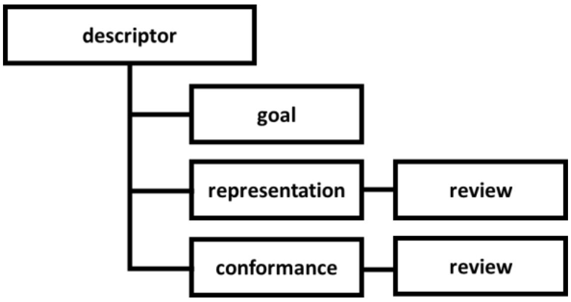


**Figure 19: Principal structure of a data quality indicator** (106)

The stated requirements, typically specified by the user, obviously have an effect on the assessment of data quality for a given study. Yet, for different indicators, this can vary, as these requirements “radiate” in a different way through the modelled life cycle.

For the location, and also for the product / the technology, the requirements will be specified by the neighbouring process in the LCA. For production processes, the requirements will be set by the process receiving the product; for waste treatment processes, the requirements will be set by the process delivering the waste.

Precision and representativeness requirements are typically valid for the entire study, as well as the modelling and support type indicators. Also, time is valid throughout the entire LCA study.

For EF, users are not entirely free in their goal and scope setting, since some elements are mandatory (the LCIA method for example), and some of the modelling options are fixed. This is the case of a partially predefined requirement set for the dataset and LCA model.

Finally, to come to an **overall data quality result** from the results obtained for the different data quality indicators, EF proposes a simple formula, basically an arithmetical mean to obtain an overall data quality rating, DQR.

$$DQR = \frac{\overline{Te_R} + \overline{G_R} + \overline{Ti_R} + \bar{P}}{4}$$

where

DQR means data quality rating,
$Te_R$ 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.

Finally, ecoinvent assumes a direct **uncertainty** influence for the different measurement data quality indicators for different scores (e.g., a 3 for geography has a specific uncertainty contribution). This uncertainty contribution is independent of the location and the technology; sources for supporting the uncertainty contribution are not documented.

### Options in data quality assessment

The first option is **whether to apply a data quality assessment** or not.

Then, the question is about which **scope of data quality** to apply:

- only for scope 1a, unit processes;
- scope 1a+1b, unit processes and elementary flows;
- scope 1a+1b+2, unit processes and elementary flows and aggregated datasets;
- scope 1a+1b+2+3, unit processes and elementary flows and aggregated datasets and study results.

A next option is about whether to **use only science-based measurement or also permit data quality obtained via the expert approach**, which is quite common in current data quality in LCA.

Further, it is to be decided which **kind of data quality indicators** are to be considered:

- only measurement;
- measurement + modelling;
- measurement + support;
- measurement + support + modelling.

A next aspect to decide is the **degree of user interaction**: users able to flexibly specify requirements, which in turn determine data quality, or bound to specific (e.g., EF) applications.

A further question is whether **uncertainty** should be reported in addition to data quality indicator results. As the link to uncertainty is not too strong, it is for now recommended not to consider the link to uncertainty for data quality.

Then, it is to be discussed whether **acknowledgement of data quality results** should be permitted. Since at present, the procedure to obtain data quality assessment results is not fully developed, it seems premature to decide about mutual recognition and acknowledgement.

Finally, about the aggregation of data quality scores, this is relevant to:

a) **Aggregation over the life cycle**. Here, it is to be decided whether the contribution of a process to a life cycle needs to be considered or not, by only counting extremes.
b) **Aggregation of various data quality indicator results**. An aggregation eases the handling of data quality results, but this point deserves more consideration. Various data quality indicators do not necessarily have the same importance for the decision, which disables a simple average calculation.

### Requirements and recommendations

**Whether to apply a data quality assessment** for LCA data or not: since LCAs are typically about decision support, and in decisions, information about the reliability of data considered is important, skipping data quality is not supported.

**Box 43. Data quality I**

Data quality must be documented and a data quality system with different data quality indicators applied.

Which **scope of data quality** to apply: since aggregated processes are in the end calculation results, it is recommended to consider data quality at scopes 1a, 1b, 2 and 3 together.

**Box 44. Data quality II**

Data quality should be considered for unit-process datasets, for exchanges, for aggregated datasets, and for calculation results and studies.

Whether to **use only science-based measurement or also permit data quality obtained via the expert approach:**

**Box 45. Data quality III**

For obtaining data quality indicator results, science-based measurements are preferred; the expert judgement approach is also permitted, due to its prevalence.

Which **kind of data quality indicators** are to be considered:

**Box 46. Data quality IV**

The data quality indicator system should be built on the UN GLAD data quality system, considering measurement, support, and modelling related indicators. This means that the system follows a pedigree table approach, with integer scores for indicator states.

The **degree of user interaction:**

**Box 47. Data quality V**

Data quality calculation must reflect user input and be calculated “on the fly” as it radiates throughout the LCA model.

About the **aggregation of data quality scores**:

**Box 48. Data quality VI**

An aggregation of data quality scores, per indicator over the life cycle, must consider the contribution of each process to the calculation results; a mere counting of extremes is not considered promising as it loses too much information.

**Evaluation: “method readiness level”**

- data quality assessment, pedigree, with user input, contribution calculation ●●●○○

**This section is linked to the following sections of the present guidelines:**

- 2: Goal of the Life Cycle Assessment
- 3: Scope of the Life Cycle Assessment
- 4.1: Life Cycle Inventory – Data sources and availability

## 5. Life Cycle Impact Assessment

### Motivation

The LCIA phase builds on the inventory and calculates the indicators representing different environmental impacts. Various methods and categories can be applied in this step, and the choices should be stated as part of the goal and scope of the LCA. Certain impact assessment methods should be preferred for FCH systems to enhance comparability, which is addressed in this chapter.

### Description of the topic

The **LCIA** phase of the LCA framework considers two mandatory (**classification** and **characterisation**) and four optional (**normalisation**, **grouping**, **weighting** and **data quality analysis**) steps. This phase considers the **Impact Assessment Method** with the selected **impact categories** to calculate the environmental impacts.

### Requirements and recommendations

#### General requirements and recommendations

**Box 49. Life Cycle Impact Assessment I**

In accordance with the goal and scope of the LCA study, the selected impact assessment method with the corresponding impact categories must be stated and justified. Compatibility between the inventory flows and the flows applied in the calculation method must be verified.

### Requirements and recommendations for FCH systems

Each impact assessment method follows its own classification and characterisation, leading to different characterisation factors for every flow/indicator. Aiming to standardise the choice of the impact assessment method, it is here recommended to use the latest version (currently version 3) of the Environmental Footprint method provided by JRC. The EF 3.0 method contains 16 default impact categories (highlighted in bold in Table 3), which must be included in the LCA study unless a reason for excluding some of them is clearly stated and justified. Therefore, the characterisation factors considered in this method (107) need to be applied. Regarding the non-default impact categories (e.g., climate change - biogenic), their application is also recommended for FCH systems.

**Table 3. Impact categories and reference units in the EF 3.0 method**

| Impact Categories | Reference Unit |
|---|---|
| **Acidification** | mol $H^+_{eq}$ |
| **Climate change** | kg $CO_{2\ eq}$ |
| Climate change - Biogenic | kg $CO_{2\ eq}$ |
| Climate change - Fossil | kg $CO_{2\ eq}$ |
| Climate change - Land use and land use change | kg $CO_{2\ eq}$ |
| **Ecotoxicity, freshwater** | CTUe |
| Ecotoxicity, freshwater - inorganics | CTUe |
| Ecotoxicity, freshwater - metals | CTUe |
| Ecotoxicity, freshwater - organics | CTUe |
| **Eutrophication, freshwater** | kg $P_{eq}$ |
| **Eutrophication, marine** | kg $N_{eq}$ |
| **Eutrophication, terrestrial** | mol $N_{eq}$ |
| **Human toxicity, cancer** | CTUh |
| Human toxicity, cancer - inorganics | CTUh |
| Human toxicity, cancer - metals | CTUh |
| Human toxicity, cancer - organics | CTUh |
| **Human toxicity, non-cancer** | CTUh |
| Human toxicity, non-cancer - inorganics | CTUh |
| Human toxicity, non-cancer - metals | CTUh |
| Human toxicity, non-cancer - organics | CTUh |
| **Ionizing radiation** | kBq U-235 $_{eq}$ |
| **Land use** | Pt |
| **Ozone depletion** | kg CFC11 $_{eq}$ |
| **Particulate matter** | disease inc. |
| **Photochemical ozone formation** | kg NMVOC $_{eq}$ |
| **Resource use, fossils** | MJ |
| **Resource use, minerals and metals** | kg Sb $_{eq}$ |
| **Water use** | $m^3$ depriv. |

**Box 50. Life Cycle Impact Assessment II**

The use of the latest version of the Environmental Footprint method is required (currently version 3.0), and all the impact categories are required. In case it is decided not to include a specific impact category, this must be justified. The characterisation factors implemented by the method provider should be checked.

Regarding optional LCIA steps, in agreement with previous FCH-specific LCA guidelines (10,16), the application of normalisation, grouping and weighting is not recommended as the opposite would decrease transparency. If normalisation, grouping and weighting are applied, it is necessary to present the results before and after the application of these optional steps. In addition, the normalisation and weighting factors are to be reported as part of the LCA documentation, justifying the reason for the selected numbers.

**Box 51. Normalisation, grouping and weighting**

Normalisation, grouping and weighting are not recommended. Still, in case they are applied, it is needed to present the results also before the execution of the optional steps. All numbers/factors considered for these calculations must also be disclosed.

An additional aspect of interest concerning FCH systems is related to the need for critical raw materials (CRMs), which has been identified as a potential barrier to its future massive deployment (108). It should be noted that LCA reveals the potential environmental impacts of economic activities (technosphere) on nature (biosphere) considering elementary flows, while criticality methods study the risks related to a product or sector due to socio-economic circumstances affecting all the stages of the supply chain. Thus, LCIA methods provide characterisation factors that are applied (only) to elementary flows, while criticality is also affected by intermediate flows appearing between economic activities in the technosphere (109). Bearing in mind the aforementioned differences, it is deemed relevant to include a separate indicator to analyse criticality (Box 52). Although this indicator is built following the LCA calculation setup (i.e., characterisation factors are proposed for each of the materials), it does not follow the same philosophical approach since the proposed factors are based on European metrics for a set of supply chains of materials.

### An approach to criticality assessment of FCH products

A combined indicator considering the Supply Risk (SR) as defined by the European Commission (110,111) and the European production of a material for consumption in the EU is recommended. It is argued that a high consumption poses a high risk if the EU relies heavily on imports of this material, and it is not recycled within the EU. The CF of each material *m* is therefore derived by:

$$CF_m = SR_m / [c_m \cdot (1 - IR_m \cdot (1 - EoL_{RIRm}))]$$

with *c* being the total European consumption of primary and secondary material, *IR* the import reliance, and $EoL_{RIR}$ the recycling input rate. Values for SR, IR and $\mathrm{EoL}_{\mathrm{RIR}}$ are provided by the European Commission (110,111) while the consumption can be retrieved from the factsheets for materials (which are updated and released every 3 years), complemented by other databases regarding secondary materials.

The criticality of each material *m* in the FCH product is given by the multiplication of the mass of the material *m* in the foreground system by its corresponding characterisation factor:

$$Criticality_m = mass_m \cdot CF_m$$

All materials considered in the EU critical material list (i.e. critical and non-critical ones) should be included. The resultant indicator should be interpreted along with the “Resource use, minerals and metals” one.

### Box 52. Critical Raw Material Assessment

Due to the particularities of FCH products, material criticality assessment is also relevant. An additional indicator is suggested according to the SH2E guidelines. This indicator:

1. is based on the Supply Risk (SR) sub-indicator divided by the import reliance and recycling rate-corrected consumption of each material.
2. must be aligned with the indicator “Resource use, minerals and metals” considered in the EF3.0 list.

All materials included in the EU critical material list are considered for the foreground system.

Due to the multidimensional scope of this criticality indicator, further elaboration on this topic might be necessary within the framework of the future SH2E LCSA guidelines.

**Evaluation: "method readiness level"**

- Selection of impact assessment method ●●●●●
- Selection of impact categories ●●●●○
- Material criticality ●●○○○

**This section is linked to the following sections of the present guidelines:**

- 2: Goal of the Life Cycle Assessment
- 3.1.1: Scope of the Life Cycle Assessment – Modelling approach - Prospectivity
- 3.3: Scope of the Life Cycle Assessment – System Boundaries

- 4: Life Cycle Inventory
- 5.1: Life Cycle Impact Assessment – Non-linearity
- 5.2: Life Cycle Impact Assessment – Risk Assessment

## 5.1 Non-Linearity

The concept of non-linearity in LCA is not univocal since literature embraces different meanings of non-linearity referring to the mathematical functions underlying all LCA input data (112):

- Goal and scope definition: functional unit/reference flow.
- Inventory analysis: product and elementary flows.
- Impact assessment: characterisation factors, normalisation factors, and weighting factors.

For the first two points, the linear assumption means that technologies are modelled as linear, so no effect of scale on production or consumption is accounted (cf. Section 3.1.1 on “learning phenomena” for further details). In other words, assuming a linear product system scaling up, the impacts associated to the production of one million units is one million times higher than producing one unit only (113). At this point, practitioners must take into account the validity of foreground and background inventory sources according to the specific features reported in them (e.g., validity of inventory data according to plant size; cf. Sections 2 and 4 on goal and data, respectively). Some authors further investigate the effect of marginal production and demand in a spatial model which involves producers and consumers across different regions (114).

The third point is more common. Traditionally, LCA assumes a linear relationship between the functional unit and the environmental impacts. In other terms, LCA characterisation factors have been estimated by assuming that an additional amount of a certain perturbation introduces marginal changes in a *ceteribus paribus* background system (115). In general, this assumption (reflected in a linear characterisation) can be used when the assessed intervention is assumed not to shift the current state to a part of the dose-response curve with different slope (116). Besides this effect, for many indicators the link between the environmental damages and the environmental emissions depends on several factors, such as fluctuations of emission rate over time, seasonal variations of environmental fate and transport processes and dose-response relationships (117). Therefore, linear characterisation and static factors might result in a too rough approximation. For instance, the human health impact from chemicals largely varies across the population depending on exposure and toxicological susceptibility. A more accurate estimation can be done using a non-linear dose-response relationship combined to heterogeneous susceptibility (118). Non-linear characterisation can also be used to account for the spatial and temporal scale of the impacts (119)**.**

Overall, the choice of introducing non-linearity in the impact assessment method and/or accounting for the scale effect largely depends, besides on data availability, on the application and scope of the specific LCA study.

**This section is linked to the following sections of the present guidelines:**

- 2: Goal of the Life Cycle Assessment
- 3.1.1: Scope of the Life Cycle Assessment – Modelling approach - Prospectivity
- 5: Life Cycle Impact Assessment
- 6.1: Interpretation and final remarks - Thresholds

## 5.2 Risk Assessment

### Motivation

An LCA is typically deterministic when it comes to evaluating potential impacts. In reality, many things happen only with a certain probability, be it accidents or failures. Further, many things addressed in an LCA are not entirely known, for example impact pathways and specific impacts. Probability is often used in scientific modelling to express this not-knowing.

There are instances where probabilistic events and not-knowing might have a larger share on the overall impact, be it accidents in nuclear power plants, explosions or leaks in FCH systems, the impact of nanomaterials on the environment, impact pathways of emissions, or future market structures.

Reverting to the original idea of LCA as a holistic approach for decision support taking into account the environmental performance of products and services, designed to prevent burden shifting, calls for an approach to include an assessment of these cases. More specifically, this calls for an approach to address the risk inherent in the options and decisions at stake, in addition to the deterministic LCA.

### Description of the topic

Risk is defined as probability of an event times the impact of this event. A classic visualisation is the risk assessment bow tie, with the probabilistic ("hazardous") event in the middle of the tie (Figure 20) (120).

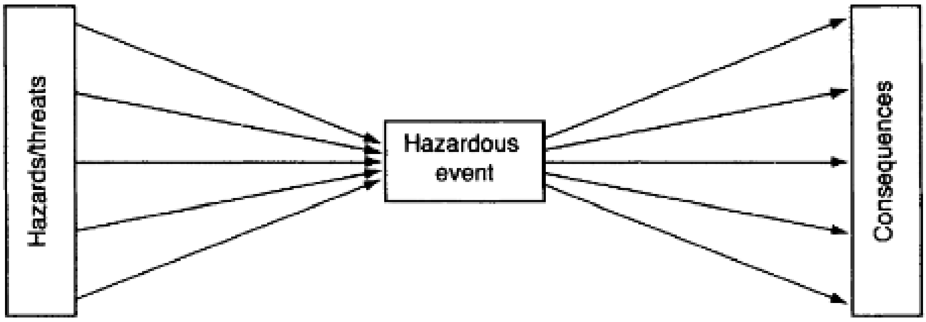
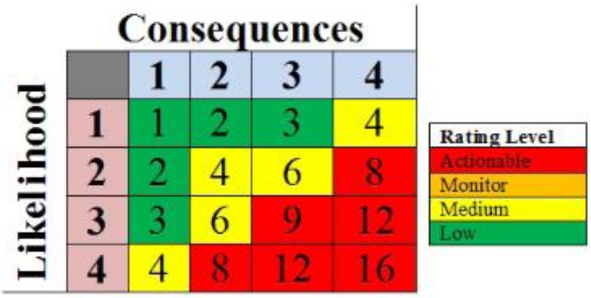


**Figure 20: Classic bow tie image of risk assessment** (120)

Risk assessment is an own discipline. In particular, qualitative or ordinal assessments of risk, using risk and probability or likelihood classes, have been proposed and used (e.g. Figure 21).



| | | Consequences | | | |
|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 |
| Likelihood | 1 | 1 | 2 | 3 | 4 |
| | 2 | 2 | 4 | 6 | 8 |
| | 3 | 3 | 6 | 9 | 12 |
| | 4 | 4 | 8 | 12 | 16 |

| Rating Level |
|---|
| 🟥 Actionable |
| 🟧 Monitor |
| 🟨 Medium |
| 🟩 Low |

**Figure 21: Qualitative Risk Assessment Matrix, with four classes of consequences and four classes of likelihood** (121)

In the context of chemical evaluation and the European REACH regulation, risk is a key term. Figure 22 shows a flow diagram to detect and check whether risk is present, in a given situation, specifically for one substance and one event. In this diagram, a risk is assumed if the predicted environmental concentration (PEC) is higher than the predicted no-effect concentration (PNEC), i.e., if the ratio PEC/PNEC is above 1. Nevertheless, this section is not limited to chemical risks, but general for issues happening only with a certain probability.

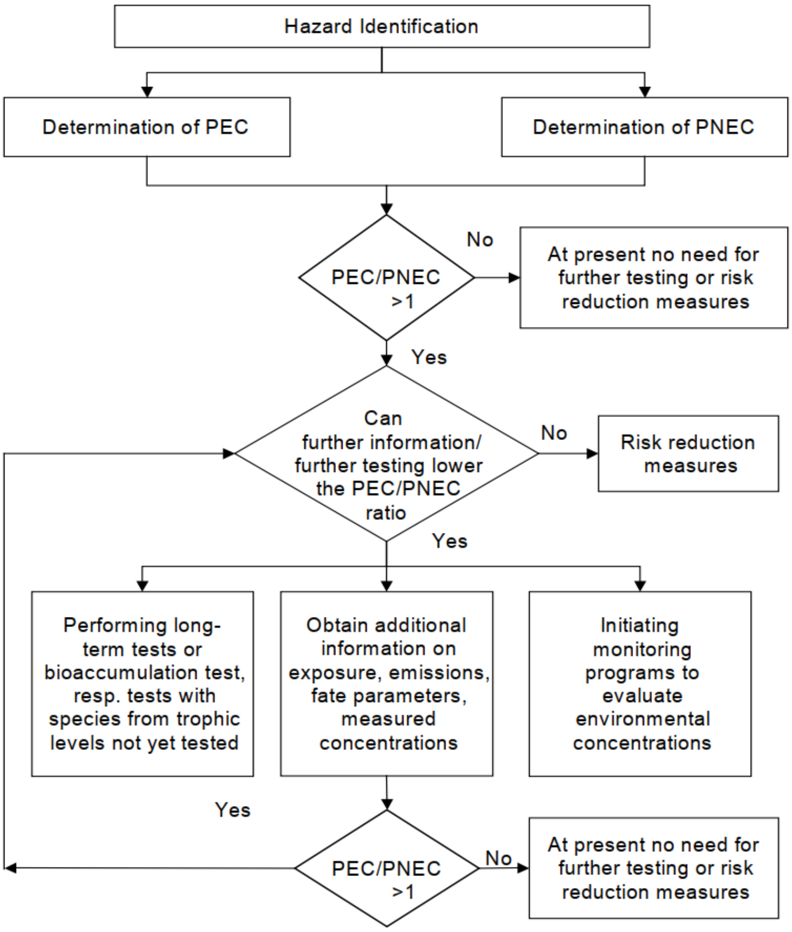


**Figure 22: Environmental risk assessment workflow (PEC: predicted environmental concentration; PNEC: predicted no-effect concentration)** (122)

## Options

The first option is **whether to apply a risk assessment (RA) with LCA** or not. If so, it is to be decided **how to apply RA**, or more precisely, how the RA that is performed is connected to the LCA, i.e. the architecture of RA and LCA. And finally**, where to apply the RA** (for which elements).

For the first question, an RA can be applied as an additional, separate modelling and assessment, not directly connected with the LCA. However, this likely leads to inconsistencies and double counting and is likely leading to more effort, as similar data collection steps are then performed for LCA and RA (123). The other option is to perform the RA connected with LCA, and here, again, there are several possibilities. For one, a detailed, risk-based foreground model can be developed, typically for one location, and supply chains are added to this model to complete the life-cycle representation, e.g. (124). Second, RA can be applied as part of a scenario modelling in LCA, where different “branches” of the life cycle inventory, for example disposal pathways, are modelled to happen with a certain probability.

An example is (125). A third option is to model exchanges with probability, as needed. These exchanges are inputs and outputs of processes, and can also be elementary flows. This approach has been developed and applied in (126).

### Recommendations

The focus is here on FCH systems, but the recommendations can be extended to other comparable systems as well.

#### Box 53. Risk Assessment I

A risk assessment is recommended when conducting an LCA of FCH systems, since accidents and other events with probability likely influence the environmental impacts of FCH systems over their life cycle.

Regarding the connection and architecture of LCA and RA, adding probability to exchanges is a flexible approach able to address both the unknown and the hazardous event. To apply it, three stages are needed:

- Identification of the processes in LCA that are to be connected with RA, by exchanges that have probability.
- Modelling of the events as LCA processes.
- Quantification of the probabilities.

Since this is a rather new approach, more public documentation needs to be made available, which is out of the scope of these guidelines.

#### Box 54. Risk Assessment II

RA should be modelled connected with LCA, using exchanges with probabilities in the LCA models.

#### Box 55. Risk Assessment III

Documentation should be provided to explain the approach of applying RA in connection with LCA via probability in exchanges.

**Evaluation: “method readiness level”**

- Risk assessment in connection with LCA, using exchanges ●●○○○

**This section is linked to the following sections of the present guidelines:**

- 3.1: Scope of the Life Cycle Assessment – Modelling approach
- 3.2: Scope of the Life Cycle Assessment – Functional unit
- 3.3: Scope of the Life Cycle Assessment – System boundaries
- 4: Life Cycle Inventory
- 5: Life Cycle Impact Assessment

## 6. Interpretation and final remarks

Beyond common practices such as sensitivity and uncertainty analyses and critical reviews (10,16), the following sections address underdeveloped (but relevant) practices when it comes to contextualising LCA results (e.g. within the scope of the Absolute Environmental

Sustainability Assessment methodology) and providing LCA practitioners with insights into the quality of their model.

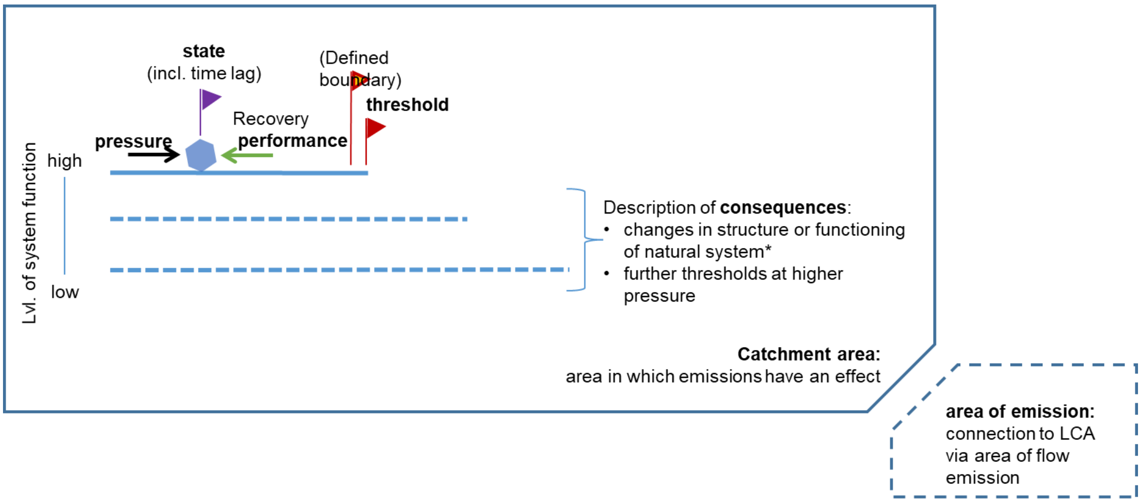
## 6.1 Thresholds

### Motivation

If a system (the earth or a more local system such as a forest) is used beyond its capacity and beyond its ability to bear the stress induced by exploiting it, it is not used in a sustainable way (127). For an LCA within an integrated sustainability assessment, this raises the question about how thresholds should be considered. For climate change, as one important impact addressed in LCA, thresholds have been determined as “tipping points”, that, when exceeded, change the entire system (128). Rockström et al. (129) introduced the planetary boundary concept, which also follows the idea of thresholds that, when exceeded, bring humanity out of a safe operating space.

### Description of the topic

The topic can be further explained through the example of northern European lowland lakes and their reaction to nutrients (130,131). In a simple model of a lake, there is detritus leading to nutrients, which are fed to phytoplankton and underwater plants, which are eaten by zooplankton, which again are eaten by fish; dead plants and fish lead to detritus. If additional nutrients are available in the lake (e.g., due to emissions from agriculture), the amount of phytoplankton increases, with the consequence of underwater light extinction and a decrease in macrophytes and zooplankton. An increase in nutrients, which can be measured as an increase in chlorophyll, changes the entire system (131). As shown in Figure 23, the goal is to know the state of the system, pressures and recovery performance, with boundaries that are “warning markers” shortly before a threshold is reached. When this threshold is exceeded, the system moves to a different overall function.



*describing chain of consequences until effect on humankind is displayed

Figure 23: Illustration of the stability of a system, with pressures, recovery performance, identified boundaries and thresholds

In order to consider and specify thresholds, the following elements and needs are relevant:

- A **system**, which is in a given **state**, and has a certain **function** that can be observed or described (for the lakes in the example above, this is the ecological status).

- It is possible to discern **levels of the state** (e.g., cyanophytes versus chrysophytes in lake eutrophication).
- The system is affected by “something” that exerts **pressure** (for the example on lakes, this could be wastewater, effluents from agriculture, and/or groundwater with nutrients).
- The system responds to pressures; ideally, this response can be expressed in a **response function** (expressing the dependency between stressors and caused impacts).
- Systems are often, to some extent, stable; they can return, after having been exposed to pressure, to the previous state. This refers to a **recovery performance** of a system.
- There may be a known **history** of previous impacts caused, as well as of previous pressures “survived” by the system.

Describing all these points in detail for a given system, let alone for all “relevant” places in a supply chain, and aggregating them over the life cycle, is typically considered infeasible. In system dynamics, stability of a system is given if a Lyapunov function can be found, which describes the conditions and thresholds for a stable system (132). However, for real-world systems, finding a Lyapunov function is an intricate problem on its own (133) and, in most cases, will not be a viable option. On the other hand, practical options for identifying thresholds in systems include simple system dynamics models and causal diagrams (134), cornerstone modelling (135,136), and –to a certain extent– consequential LCA (Section 3.1.2). These options can also be combined.

**Simple system dynamics and causal diagrams**

This option follows the idea of Bossel (134), which can be summarised as follows:

- First, characterise a system by creating a “word model” for the system. This model describes, in simple sentences, the function of the system, the main elements and their direct relations. Mention thresholds of system values, pressures and impacts, as long as they are known.
- Second, create a qualitative diagram (often called causal loop diagram) that shows these main elements from the text with their relations, with the direction of the impact of one element on the other displayed. It is very useful to add “+” or “–” to the connecting relations in order to distinguish enforcing relations from damping ones. This has been applied by, e.g., Di Noi and Ciroth (137). Closed feedback loops that are containing either only damping (-) or only reinforcing (+) relations deserve special attention, as they indicate “spots” where the system may go out of balance and thus exceed thresholds. Chains of relations are also interesting, since they allow deducing impacts and connections between remote elements.
- Third, quantify this diagram, most likely not in its entirety but partially. In an ideal case, for modelling the environmental impacts of a product over its life cycle, a large area in the diagram can be reflected by a linear LCA model. Where the linear model is not valid any more, a different model is to be used, which could also be linear.

It is useful to perform these models for three parts of the LCA: resources, technosphere (i.e., product supply, use, and end-of-life network), and emissions. Depending on the case, additional, more focused, models can make sense. However, it is recommended to start with an overarching, general model for a problem, and then identify spots that potentially need more detail.

### Cornerstone scenarios

Cornerstone scenario modelling is a technique where, for a given hard-to-grasp system such as future energy uses and production, several key, distinct and rather extreme cases are modelled, with the idea that the real state of the system will probably lie in between these modelled extremes (135,136). This can be useful to extend the validity of modelling results, without the need to model a continuous area of possible cases. For instance, Spielmann et al. (136) used this approach to model the environmental impacts, over the life cycle with rebound effects, caused by a planned future high-speed train in Switzerland.

## Recommendations

In general, the consideration of thresholds is recommended, though beyond current LCA practice. It is especially useful when modelling systems not fully understood, such as new technologies or systems which will potentially hit thresholds (scarce resources, tight markets and supplies, restricted uptake of waste, or impacts exceeding the bearing capacity and recovery performance of the natural environment). In particular, FCH systems currently face market constraints, their impacts are not entirely certain, and the required infrastructure and components use some resources classified as critical or scarce. Hence, for FCH systems, it is recommended to create system dynamics and causal loop diagrams before modelling the life cycle in a linear way, using LCA.

### Box 56. Thresholds

1. For a system that is about new technologies or otherwise containing major parts that are not yet fully known, or for systems that potentially hit thresholds, it is recommended to create system dynamics and causal loop diagrams before modelling the life cycle in a linear way, using LCA.

2. If thresholds and loops are detected in the system dynamics model, the LCA should address these by clearly identifying its own validity space, within these thresholds, or by combining different models with a different validity space.

**Evaluation: “method readiness level”**

- System dynamics integration in LCA ●○○○○
- Cornerstone modelling ●●●○○

**This section is linked to the following sections of the present guidelines:**

- 2: Goal of the Life Cycle Assessment
- 3.1: Scope of the Life Cycle Assessment – Modelling approach
- 3.3: Scope of the Life Cycle Assessment – System boundaries
- 5: Life Cycle Impact Assessment

## 6.2 Verification and validation

### Motivation

Since any LCA is a model of the life cycle of the object under study, it is important to understand how “good” this model is.

### Description of the topic

Reality itself is a highly complicated concept (138). Here, reality can be understood as “*the state of things as they actually exist, as opposed to an idealistic or notational idea of them*” (139). In this regard, an LCA is a model of the life-cycle impacts of a product in reality.

Verification is known in modelling theory as checking whether a model is technically built correctly ("building the model right"), while validation is understood as checking that the model does what it is supposed to do ("building the right model") (140). Hence, model validation is a topic of fitness for purpose and thus data quality. Verification is then the task to check that the LCA model, in line with its goal and scope, really models the life cycle that is intended, which includes that the model is supported with "real" data.

## Options

In order to investigate how well a given LCA model or parts of it represent reality, a number of options are available, and different cases and settings can be distinguished.

**The first is a fully rule-based approach**. In this approach, rules are defined, and it is checked whether these rules are applied correctly, on a practical case. For these checks, applied procedures "in reality" are compared against the defined, approved rules, and checked for compliance (Figure 24). These checks may sometimes be referring to and addressing the initial goal, while other times it is merely checked that a rule is fulfilled. Looking at LCA, there are often rules defined to ensure the quality of the LCA and its results. For example, the PEFCRs document by the European Commission (2) contains specific rules for modelling different types of processes and products, life-cycle stages, and the share between different connected life cycles.

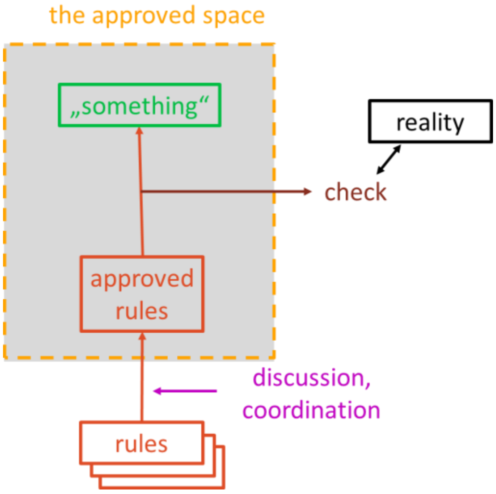


Figure 24: Rule-based approach

The second option is **a fully empirical approach**. In this option, the model receives direct input and feedback from real data, which is used to adjust and adapt the model results (potentially also the model structure). A number of approaches are used, ranging from statistical methods to neural networks that are trained with real data (Figure 25). This approach has a long tradition in modelling and is the basis for model-based learning and artificial intelligence (141). For LCA, not all data and not all results can be fully taken as real data. For instance, it is not possible to obtain the whole carbon footprint of a product system as real data (142). For this reason, this approach alone cannot actually be used for LCA.

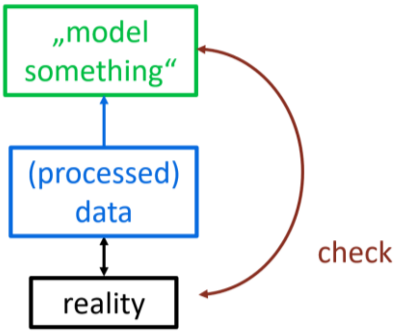


Figure 25: Empirical approach

The **third option is a hybrid approach**, where some elements are taken from a real system, and some are obtained based on rules. In this hybrid approach, the degree of real data used can vary. In LCA models, data to be used in a model are often approved as well, in addition to rules, and thus become part of the approved modelling space.

Overall, for common uses of LCA data and for popular and broadly discussed LCA quality assurance systems, the degree of real data (and of considering reality) is typically low. In fact, it is not current practice in LCA to check whether an LCA model or parts of it represent reality, with some exceptions (143). The hybrid approach in LCA can be summarised as follows (Figure 26): modelling rules are established, often following a standard, sometimes also following more detailed rules for specific product groups (e.g., the product category rules in the PEFCR specific documents); data are identified that conform to the defined rules; and LCA models are built following the rules, using the recognised, conforming data as building blocks. As an additional layer of assertion, a review is often performed for data and also for the models.

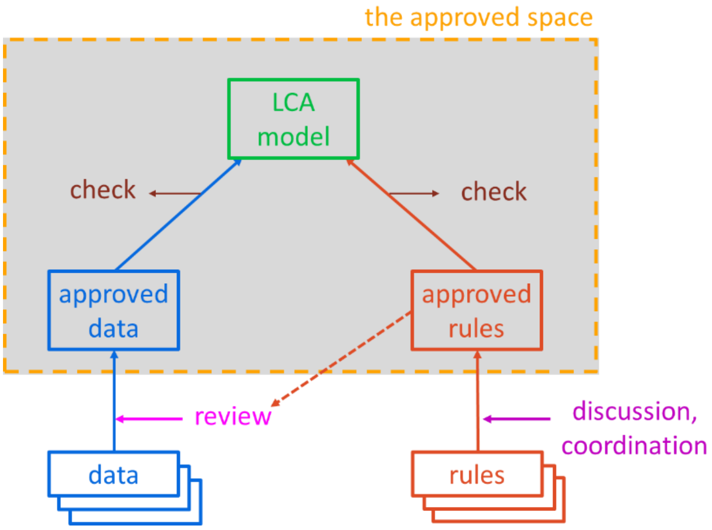


Figure 26: Hybrid approach

## Requirements and recommendations

At present, LCA models do not typically benefit from the advantages of real data. However, there are several possibilities, at different levels, to include real data and a “reality feedback” in LCA models. For instance, at the assessment level, the evaluation about whether and how far rules are met and data are compliant can be performed automatically and unsupervised, or by one person or several people. It can be designed so that the assessment can be repeated, making the object of investigation accessible.

Regarding the topics addressed in the review, the review can check and investigate many different aspects of an LCA model: single inputs or outputs, input/output relations, full processes, local impacts caused, global impacts caused, emissions occurring, market shares, modelling rules followed, learning curves (as far as important for the model), etc.

Regarding the observability of results, there are different levels: direct observation; derivation, second order (e.g., water shortage because of change of vegetation in a certain area); and otherwise concluded information, based on e.g. probability. Concerning the result that is observed, it can be quantitative or qualitative.

Overall, it is not easy to verify and validate an LCA in total. Although each verification step can be partial, overall the verification steps ideally complement each other. For the overall management of the verification, it is recommended to develop pedigree tables.

**Box 57. Verification and validation I**

The LCA model should be a hybrid model, with data and rules being partially supported by real data.

**Box 58. Verification and validation II**

An LCA model that has important support from real data is preferred. Real data should be reflected not only in review criteria but also during the reviewing process.

**Evaluation: “method readiness level”**

- Verification ●●○○○

**This section is linked to the following sections of the present guidelines:**

- 3: Scope of the Life Cycle Assessment
- 4.2: Life Cycle Inventory – Data quality

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