

LCA4CCU

Guidelines for Life Cycle Assessment of Carbon Capture and Utilisation

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1 Executive summary

Carbon Capture, Utilisation and Storage (CCUS) is perceived as one of the options available to address the hardest-to-abate emissions from process industries such as iron & steel, cement and chemicals, which are heavily carbon-intensive. CCUS includes storing CO₂ in geological formations (for example in a deep saline aquifer) as well as its use in processes for conversion into chemical products, building materials or fuels. The largest benefits of CCUS in literature are mostly from the geological storage (CCS), while the potential benefit of utilisation options (CCU) is still under investigation. In this report, the focus is only on the capture and use of CO₂ as raw material in conversion processes, although the guidelines and principles can be applied to CO₂ used in other processes.

This report aims, within the framework provided by DG Energy, to develop Life Cycle Assessment (LCA) guidelines for Carbon Capture and Utilisation. As a point of departure, CCU is defined in this report as “those technologies that use CO₂ as feedstock and convert it into value-added products such as fuels, chemicals or materials”. CCU involves a number of stages, from capturing the CO₂ to its conversion into carbon-containing products, further including the use of such products up to their disposal as carbon-containing waste and/or ultimately, CO₂ emission, which may happen shortly after the use of the CO₂-derived product (e.g., synthetic fuels) to decades (e.g., for polymers) or centuries (e.g., for mineralization products). Many of these stages demand energy, not only directly (in the capture system and the transformation processes) but also indirectly (in the synthesis of co-reactants such as hydrogen). The products will then be used in other chains.

Understanding the potential benefits or impacts on the environment, requires that not only the direct impacts from the CCU production facility are considered but also the impacts from provision of feedstock and from use and end of life of products. Furthermore, impacts (or benefits) are not restricted to those of climate change but should also include other environmental aspects (land use, water use, etc.). As a consequence, CCU’s beneficial or negative impacts should be assessed from a system perspective and with regards to how it can provide societal benefits.

The principles of LCA are already described in ISO 14040 and 14044, and so the purpose of this work is not to revise these principles. The report does not aim to replace existing standards (e.g., EN ISO 14040 and EN ISO 14044), rather it departs from the standards and existing state-of-the-art knowledge in LCA to address points that are particularly relevant for CCU. In doing so, the objective of the report is to identify and highlight the most “controversial” topics when applying LCA to CCU technologies. Whenever possible, recommendations are made for each step of an LCA: goal and scope (functional unit and system boundaries), reference systems, data and models, impact categories and uncertainty analysis. Uncertainty is not exclusive of LCAs of CCU. However, as most CCU technologies are currently at an early stage of development (e.g., lab-scale), outputs from LCAs addressing those technologies have inherently large(r) uncertainties. Therefore, a discussion on the impact of uncertainty is also part of this work.

Main recommendations:

The key strength of LCA is that the methodology can be applied to address the environmental aspects and potential environmental impacts throughout the life cycle of *any* good or service. Given this wealth of possibilities, it is, however, very important to precisely describe the research question to be answered. This may seem a trivial point, but a review of LCA literature on CCU concepts already indicates that this point is sometimes overlooked or forgotten throughout the study (i.e. implications of a given goal setting at the start of the study do not match the methodological choices or conclusion drawn from the study). Since the goal definition is decisive for all the other phases of the LCA, a clear initial goal definition is crucial for a correct later interpretation of the results. It is thus recommended to pay particular attention to the goal definition since it affects the results and also the comparability of LCA studies. The present guidelines are intended to cover “decision support” situations according to the ILCD Handbook; therefore

“accounting” cases are out of scope of the present guidelines.

The present guidelines require that “cradle-to-grave” **should** be the default system boundary to assess the environmental impact of a CCU technology. Only in this way, meaningful conclusions regarding carbon neutrality/negativity can be drawn in an unrestricted form. Other system boundaries are discouraged (“cradle-to-gate”) or even strongly discouraged (“gate-to-gate”); however, they **may** be chosen on the condition that a justification is provided and that the conclusions drawn from the study do not (explicitly or implicitly) expand or cover issues that can only be done with larger system boundaries.

The selection of the reference system plays an important role for understanding the potential environmental benefits (or pitfalls) of a CCU option. Because many CCU options are currently at low TRL level, the selection of a proper reference system remains challenging. In this guideline, we recommend that more than one scenario **shall** be explored (such scenarios can include various reference systems, various backgrounds, etc.). Selecting only a single future scenario (e.g., novel technology vs today's technology) runs the risk of over- (or under-)stating uncertainties that are identified as well as producing blind spots. When defining the scenarios, care should be taken that they are both temporally and spatially consistent.

Regarding the impact categories, in this guideline, we use CML Impact Categories, but other categories may be used. It **shall**, however, be clear and explicitly reported which impact categories are used, including the name of methodology, version, and date released. Because one of the key values added by LCA is the potential to identify trade-offs among categories, here we recommend that all impact category types **should** be used, and if not, justification **shall** be given. Although the motivation of CCU often lies in climate change and therefore many studies focus only on indicators related to greenhouse gases (e.g., Global Warming Potential), it is important for proper decision making to identify potential areas where trade-offs can occur as a consequence of CCU implementation. Furthermore, when looking at GWP, to understand short- and long-term impacts, it is recommended that both GWP20 and GWP100 **should** be used. Finally, in this guideline we recommend that delayed emissions less than 500 years **shall** be treated as emitted at year zero, emissions delayed greater than 500 years (to a reasonable level of certainty) **should** be ignored.

In this guideline, we further recommend that system expansion **shall** be used. Sometimes, however, allocation procedures are required, and as such allocation of CO₂ is one of the most relevant topics in LCA for CCU and also a potential pitfall. Very strict compliance to guidelines is essential along with very clear communication of selected procedures at distinct places within the LCA and an assessment of the impact of allocation choices as part of the uncertainty analysis. Particular care should be taken to avoid that inadvertently emissions 'disappear' from the system, for instance, by assuming that emissions are accounted for by a party that is outside the system boundaries. In this guideline, we depart from a precautionary principle, which says that if the origin of the CO₂ to be used in the CCU options is not known or if the origin is known but there is no agreement on who has the burden of the emissions due to CO₂ capture and transport, the CCU system **shall** incorporate those into its system boundaries. Note that unless there is specific information about the source of the CO₂, it **shall not** be assumed that the flow is of non-fossil origin (i.e. CO₂ is considered of fossil origin unless information is provided which justifies to consider it biogenic or atmospheric).

Regarding impacts of (background) data, electricity tends to be much more relevant for most CCU applications than for others. Refinement compared to standard LCA is strongly recommended to improve quality of LCA for CCU, especially, it is important to consider impact of flexible operation on plant model and foreground data (e.g., if the system is assumed to use only intermittent renewables or is considered to provide an energy storage service to the grid); to further apply additionality and marginal electricity concepts, time-resolved data and to consider location of CCU plant and related potential grid restrictions.

Finally, uncertainty analysis remains an indispensable part of LCA and even more so for LCA of technologies that are not yet commercial. We recommend that whenever possible, a combination of quantitative and qualitative uncertainty methods should be used as they provide specific insights into the types of uncertainties and their significance in the analysis and that as a minimum, any LCA of CCU **should** provide a thorough report of uncertainties (in data, models, allocation choices, etc.) regardless of whether they can be (quantitatively) measured.

To conclude, no general gaps in LCA methodology were identified in application to CCU. Instead, it showed that also for CCU, LCA is THE tool of choice for assessment of environmental impacts of technologies. Nevertheless, some topics are recommended for future work in the context of LCA for CCU to accelerate the adoption of recommendations made within this report and to improve familiarity within the LCA community:

- To develop and provide examples of LCA for selected CCU cases as best practice references. In this context, examples with high relevance, either because of the absolute amount of CO₂ emitted by the respective kind of source or because of the product market size (e.g., fuels, olefins, methanol, BTX aromatics, urea) could be of special interest.
- To validate applicability of the guidelines of this report also on example cases of other, chemical energy containing gaseous components such as hydrogen or carbon monoxide which may come along with a CO₂ containing waste gas (as for example in steel mill waste gases) and - if meaningful or necessary - to expand the scope and/or add specific recommendations to the guidelines.
- To elaborate higher frequencies of background data updates and validations. This includes especially the mandatory use of most recent IPCC figures for any LCA for CCU.
- To support well defined and accepted scenarios for selected reference systems as the background system will change so fast in the coming years, though at relatively high uncertainty, to enable efficient execution of LCA as well as comparability of LCA studies by practitioners. Those reference systems should include the power system in general (including share and location of renewables, kind of renewables, level of grid development, time-dependent resolution of power production and general demand) as well as state-of-the-art for selected key industrial processes, e.g., for steel, glass and cement making and production of selected base chemicals for selected points in time, e.g., by 2030, 2040 and 2050.
- To develop and to make available background data for carbon capture technologies due to its relevance for LCA for CCU. Improvement regarding both quality and quantity of data in this area is strongly encouraged.
- Due to the relatively high number of low TRL cases among CCU technologies, it is recommended to generally foster experience with treatment of uncertainty within LCA. Uncertainty, in general, is not a specific issue of CCU technologies. Yet, its relevance is in tendency higher in the area of CCU. The common level of understanding and experience could be improved by dedicated research as well as a general stronger emphasis in future LCA.
- To develop LCI databases for CCU systems in order to support practitioners in the development analysis of CCU.

The focus of this work has been on LCA aiming to support decision making. In the case of LCA aiming for accounting it may be desirable to apply allocation instead of system expansion which could cause different results. There is no simple rule available today how to avoid such potential mismatches. It remains in the responsibility of the LCA practitioner to be aware of such differences and to consider them adequately in the interpretation of the results. Additionally, it might be useful to elaborate on selected examples of how such mismatches could be avoided or at least to provide a guideline on how to deal with it.

Beyond these recommendations, there are topics which fall out of the direct scope of LCA for CCU and/or require inclusion of additional expertise, nevertheless, it is anticipated that proper solutions would be of high value to ensure good fit between real operation of CCU plants and results from their respective

models within an LCA study. For example, it would be meaningful to provide operators of CCU plants which are designed and intended to operate only in selected situations for marginal grid mix (e.g., at sufficiently low carbon footprint), with an online tool which enables them to predict within reasonable certainty the marginal mix over a reasonable period of time in the future (e.g., up to a day ahead). Also, it is to be clarified how - in the context of additionality - renewable power plants shall be treated which fall out of the regime of any public funding scheme but which will need some investment in refurbishment prior to continued use. Neither treatment as additional renewable power nor as already fully existing renewable power installation seems adequate. Further topics may come up within the context of future application of LCA for CCU.

Finally, especially in the context of meso-/macro-level decision support by LCA and furthermore in cases which strongly rely on use of renewable electricity, it would be very meaningful to develop guidelines for how to assess the impacts of a large scale deployment of the respective CCU technology. Specifically, it would be very useful if information such as total renewable electricity demand, required transmission grid capacities, area demand for renewable power generation and transmission lines, impact of CCU plants and additional renewable power installations on availability of renewable power for other applications would be consistently developed and analysed in order to reflect future potential competition for renewable electricity, land use and grid capacity with other sectors.

Further issues which fall out of the scope of LCA for CCU specifically, but are important, are the issues highlighted in terms of the inconsistencies over the method used for climate change impacts, both the version issue (TAR, AR4, or AR5) and also the application of these methods. There needs to be greater work between LCA practitioners and the IPCC to resolve this issue.

2 Introduction

2.1 Background

Today, more than 220 Mt carbon dioxide (CO₂) are used globally each year¹. The largest consumer is the fertiliser industry, which consumes 100 Mt CO₂ per year for urea manufacturing (of which the vast majority is produced upstream by natural gas steam reforming), followed by the oil sector at nearly 80 Mt CO₂ for CO₂ Enhanced Oil Recovery (CO₂-EOR). Other commercial applications include food and beverage production, metal fabrication, cooling, and fire suppression; CO₂ is also used in greenhouses to stimulate plant growth.

A potential benefit of Carbon Capture and Utilisation (CCU) is the substitution of fossil-based products. In the chemical industry, greenhouse gas (GHG) emissions of catalytic chemical processes are dominated by the top large-volume products² (see Figure 1). The substitution of these fossil-based products could increase the market potential of CCU. The benefits in terms of GHG emissions will, however, depend on the carbon footprint of the energy used for the CCU process, the carbon emitted in the upstream and downstream processes and the lifetime of the product it replaces.

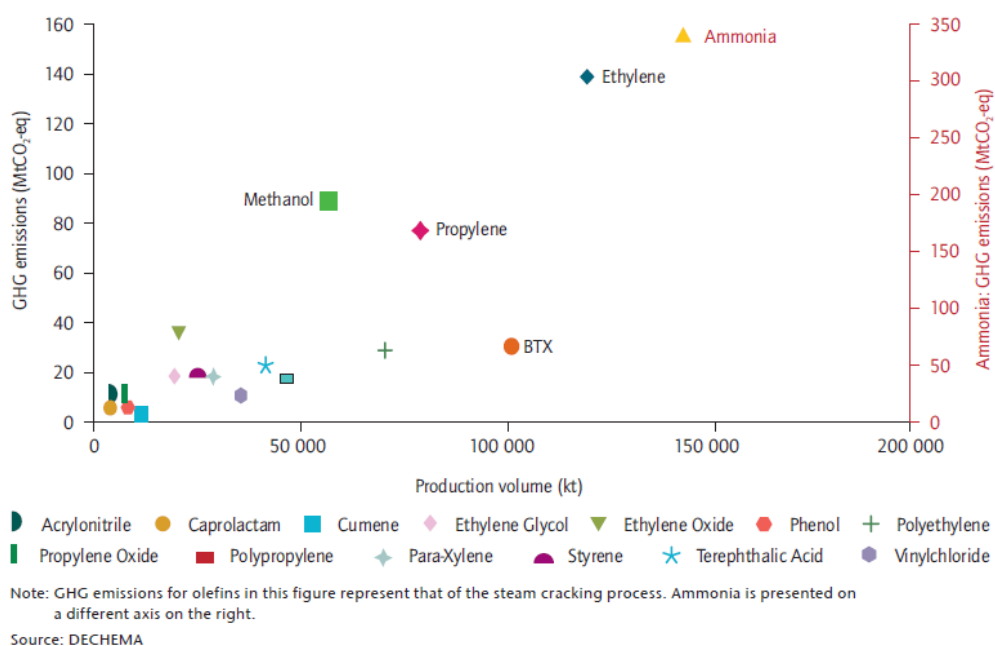


Figure 1: Global GHG emissions versus production volumes of top 18 large-volume chemicals, 2010 (Source: IEA, ICCA & DECHEMA³)

CCUS, Carbon Capture, Utilisation and Storage, is perceived as one of the options available to address the hardest-to-abate emissions from process industries such as iron & steel, cement and chemical industries, which are heavily carbon-intensive. Globally, industrial carbon dioxide (CO₂) emissions have increased by

¹ Transforming Industry through CCUS, IEA, May 2019

² Technology Roadmap “Energy and GHG reductions in the chemical industry via catalytic processes”, IEA, ICCA & DECHEMA, 2013

³ Ibid.

70% between 1990 and 2017⁴, making the industry the second-largest source of CO₂ emissions. With one-quarter of industrial emissions related to non-combustion process emissions such as chemical reactions, CCUS is considered by some as unavoidable and a cost-effective option for the future to reduce emissions from industrial processes. CCUS includes CO₂ geologically stored (for example in a deep saline aquifer) or used in processes for conversion into chemical products, building materials or fuels. The largest benefits of CCUS in literature are mostly from the geological storage (CCS), while the potential benefit of utilisation options (CCU) is still under investigation. In this report, the focus is only on the capture and use of CO₂ as raw material in conversion processes, although the guidelines and principles can be applied to CO₂ used in other processes.

Carbon dioxide, CO₂, is a molecule at a very low energy level and with high thermodynamic stability. Therefore, it typically needs considerable energy input for its conversion into a product. Other raw materials could be used as co-reactant for CO₂ (e.g. hydrogen) to enable the conversion at milder (temperature, pressure) conditions. Such co-reactants however also require energy and materials for their production. Therefore, it is crucial to assess the life cycle impact of CO₂ capture and conversion processes to identify the potential benefits and trade-offs of these new technologies.

This report aims, within the framework provided by DG Energy, to develop Life Cycle Assessment (LCA) guidelines for Carbon Capture and Utilisation (CCU). As a point of departure, **CCU is defined in this report as “those technologies that use CO₂ as feedstock and convert it into value-added products such as fuels, chemicals or materials”**.

CCU involves a number of stages, from capturing the CO₂ to its conversion into carbon-containing products, from the use of such products to their disposal as carbon-containing waste, and ultimately, CO₂ re-emission, which may happen shortly after CO₂ conversion (e.g. synthetic fuels) to decades (e.g. for polymers) or centuries (e.g. mineralization products). All these stages demand energy, not only directly (in the capture system and the transformation processes) but also indirectly (in the synthesis of co-reactants such as hydrogen). The products will then be used in other chains. Understanding the potential benefits or impacts onto the environment, requires that not only the direct impacts from the CCU production facility are taken into consideration but also the impacts due to feedstock requirements and end of life. Furthermore, impacts (or benefits) are not restricted to those of climate change but should also include other environmental aspects (land use, water use, etc.). As a consequence, CCU's beneficial or negative impacts should be assessed from a system perspective and with regards to how it can provide societal benefits.

Various studies have attempted to identify which societal services CCU could provide. Among the most named ones are:

- Long-term energy storage into chemical bonds (from intermittent renewable energy);
- CO₂ as an abundant feedstock that could increase feedstock security of industrial sectors;
- Improving the sustainability of industrial processes (green chemistry),
- A potential pathway to implement circularity in industrial systems.

This approach, based on societal services, is new and could lead to misinterpretations when applying a full LCA for a CCU technology. It is why, here, a systematic discussion of aspects for the application of LCA specifically for CCU technologies is described.

The principles of LCA are already described in ISO 14040 and 14044, and so the purpose of this work is not to revise these principles. *The objective is to identify and highlight the most “controversial” topics when applying LCA to CCU technologies.* When possible, recommendations are made for each step of an LCA: goal and scope (functional unit and system boundaries), reference systems, data and models, impact categories and uncertainty analysis. Uncertainty is not exclusive of LCAs of CCU. However, as most CCU

⁴ Exploring Clean Energy Pathways - The Role of CO₂ Storage, IEA, July 2019

technologies are currently at an early stage of development (e.g. lab scale), outputs from LCAs addressing those technologies have inherently large uncertainties. Therefore a discussion on the impact of uncertainty is also part of this work.

This document focuses on how to handle the specificities of LCA for CCU. It provides additional requirements and guidelines for CCU products:

- Chapter 3 introduces the terms used in the report and gives a definition of CCU technologies as a framework for this study.
- Chapters 4 through 8 follow the different phases of LCA and provide guidance specifically for LCA for CCU.
- Chapter 9 focuses on the description of the studied system, i.e. CCU system (what information should be used for the assessment) and the reference systems with the methodology for the choice of technology
- Chapter 10 presents key elements on data and models aspects. Also, impact categories are discussed in the chapter.
- Chapter 11 provides technical information on selected feedstock- and energy-related aspects. The assumptions made by the practitioner on these elements may have major impacts on the result of the assessment.
- Chapter 12 provides details regarding the selection of impact categories.
- Chapter 13 carries out an analysis of the impact of uncertainty on the result of the assessment. Even if uncertainty analysis is not specific to CCU technologies, it is a main point in the interpretation of the results of LCA.
- Chapter 14, the last one, summarises the main recommendations and gives an outlook on potential next steps of this work.

2.2 Context

This document is a set of guidelines for the Life Cycle Assessment (LCA) of Carbon Capture and Utilisation (CCU), to identify and, when possible, address some of the key challenges when developing LCA of CCU.

The work departed from a review of the literature regarding LCA methodology and the application to CCU. Although a significant amount of scientific work on LCA for CCU, especially on case studies, is increasingly available, there is still a lower level of experience and expertise in case of LCA for CCU and several challenges exist in selecting adequate assumptions and methods because specific boundary conditions in CCU chains often have a higher impact than in other areas of LCA application.

The general description of Life Cycle Assessment is defined in EN ISO 14040:2006. This report is based on the standards EN ISO 14040 and EN ISO 14044.

Based on the above, in summary, our points of departure are:

- This document was developed from a purely scientific perspective, free from policy and economic considerations, in order to cover all possible routes and products.
- The document is built on existing and undisputed state of the art in LCA.
- The document should support the identification of potential pitfalls and limitations within LCA for CCU and prioritize such issues.
- The document aims to provide first recommendations to overcome key issues. The LCA recommendations should be applicable by practitioners.
- The document should highlight where LCA for CCU differs from other cases of LCA, we are not recreating all of LCA.

- As a key principle of LCA, transparency is required, whilst respecting intellectual property protection by partners.

2.3 Approach

This document has been produced by a group of 7 experts from different areas of expertise but with a track record on LCA. This document was created through an extensive review of the literature regarding LCA methodology and its application to CCU. The first step was to identify the main pitfalls and limitations within LCA for CCU and prioritize such issues. A workshop gathering LCA experts was organised in May 2019 to present and discuss the identified pitfalls and limitations. Feedback from the participants was also requested. Then, the main work focused on producing recommendations to overcome the identified issues. A second workshop gathering a larger number and type of stakeholders was organised in July 2019 to present the main outcomes of the work. Proposed recommendations were discussed with the audience. After the workshop, the main recommendations were finalised. The work was based on an iterative approach with feedback from stakeholders. Also, the outcomes of the work are presented in the report.

2.4 Normative references and references to LCA guidelines

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

- EN ISO 14040:2006, Environmental management - Life cycle assessment - Principles and framework
- EN ISO 14040:2006, Environmental management - Life cycle assessment - Requirements and guidelines
- EN ISO 14067:2018, Greenhouse gases - Carbon footprint of products - Requirements and guidelines for quantification
- European Commission: International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment - Detailed guidance. First edition March 2010. EUR 24708 EN. Luxembourg. Publications Office of the European Union; 2010
- European Commission: PEFCR Guidance document - Guidance for the development of Product Environmental Footprint Category Rules (PEFCRs). Version 6.3, May 2018.

3 Terms and definitions

For the purposes of this document, the terms and definitions given in EN ISO 14040:2006, EN ISO 14044:2006 and the following apply.

To simplify the reading of the report, we make use of typical “standardisation language”: The requirements / provisions in this document are marked as either “shall”, “should” or “may” to identify the provisions’ requirement status:

- **“shall”**: the provision is a mandatory requirement and must always be followed, unless for specifically named exceptions, if any.
- **“should”**: the provision must be followed but deviations are permissible only if, for the given case, they are clearly justified in writing, giving appropriate details. Reasons for deviations can be that the respective provision or parts of it are not applicable, or if another solution is clearly more appropriate. If the permissible deviations and justifications are restricted, then these are identified in the context of the provision.
- **“may”**: the provision is only a methodological or procedural recommendation. The provision can be ignored or the issue can be addressed in another way without the need for any justification or explanation.

NOTE: Instead of "may" the term "recommended" is sometimes used and equivalent.

3.1 Definition of CCU

CCU for Carbon Capture and Utilisation has been defined for the scope of this study as “those technologies that use carbon dioxide (CO₂) as a feedstock and convert it into value-added products such as fuels, chemicals or materials.”

Along with CO₂, alternative carbon sources and/or energy carriers may be present in feed gases, especially in flue gases, which have been or might be perceived in the wider context of CCU, e.g.,

1. Carbon monoxide, CO (e.g., coking gas, blast furnace gas, converter gas),
2. Methane, CH₄ (e.g., coking gas, chemical process off-gases, flare gas, mining gas),
3. Low weight olefins (e.g., ethylene, propylene from chemical process off-gases),
4. Syngas (CO/H₂) (e.g., coking gas, blast furnace gas, chemical process off-gases).

In the scope of this work, the carbon source of CCU is restricted to CO₂ from process gases and flue gases (fossil or biogenic) or CO₂ from the atmosphere. However, the guidelines presented in this work can be applied to other carbon compounds in other off-gases (such as those produced from process emissions in the iron & steel, cement and chemical industries).

3.2 The CCU system

In CCU systems, CO₂ is considered as a raw material. The first use of CO₂ is the direct use for its physical properties as a solvent or a working fluid (physical properties). This application is one of the main utilisations of CO₂ today. CO₂ can also be used as a source of carbon, as there are many carbon-containing chemical products that could be synthesised via CCU. Chemical or biological processes can transform CO₂ into different products such as synthetic fuels (liquid or gaseous), chemical commodities and chemical building blocks, building materials or food products. Figure 2 below shows examples of the main uses of

CO₂ with or without conversion.

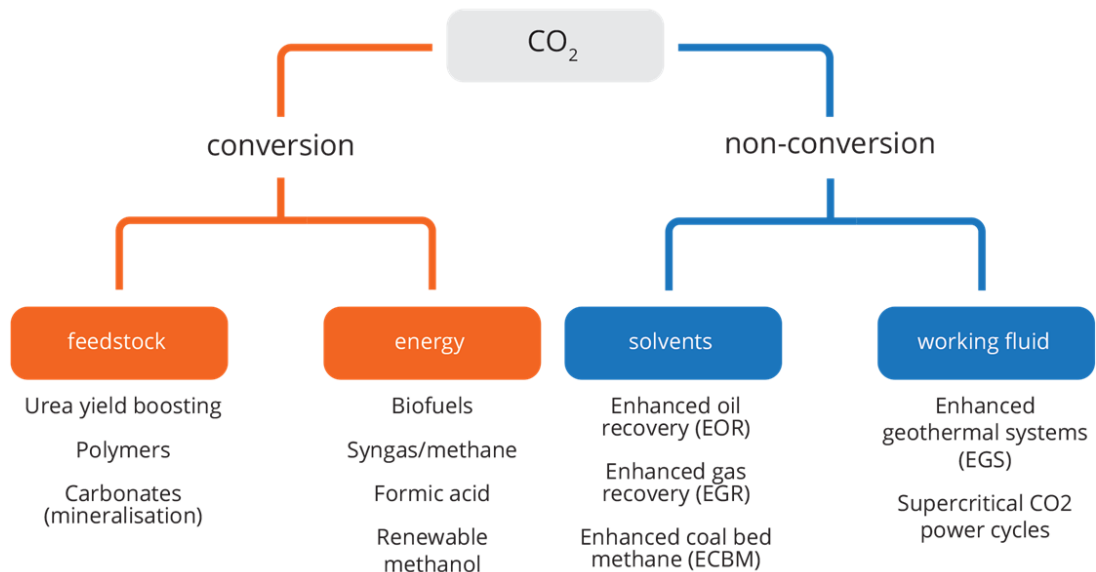


Figure 2: Simple classification of CO₂ uses (Source: IEA⁵)

The range of potential CO₂ uses/applications is very large and includes the intermediate use by which the CO₂ is not chemically altered and the use of CO₂ by conversion into a product. Most of today's industrial applications are based on the direct use of CO₂, such as for greenhouses, carbonated beverages or enhanced oil recovery (EOR). However, the largest demand of CO₂ today is for the production of urea (100 Mt of CO₂). Figure 3 below illustrates the different options for a CCU system.

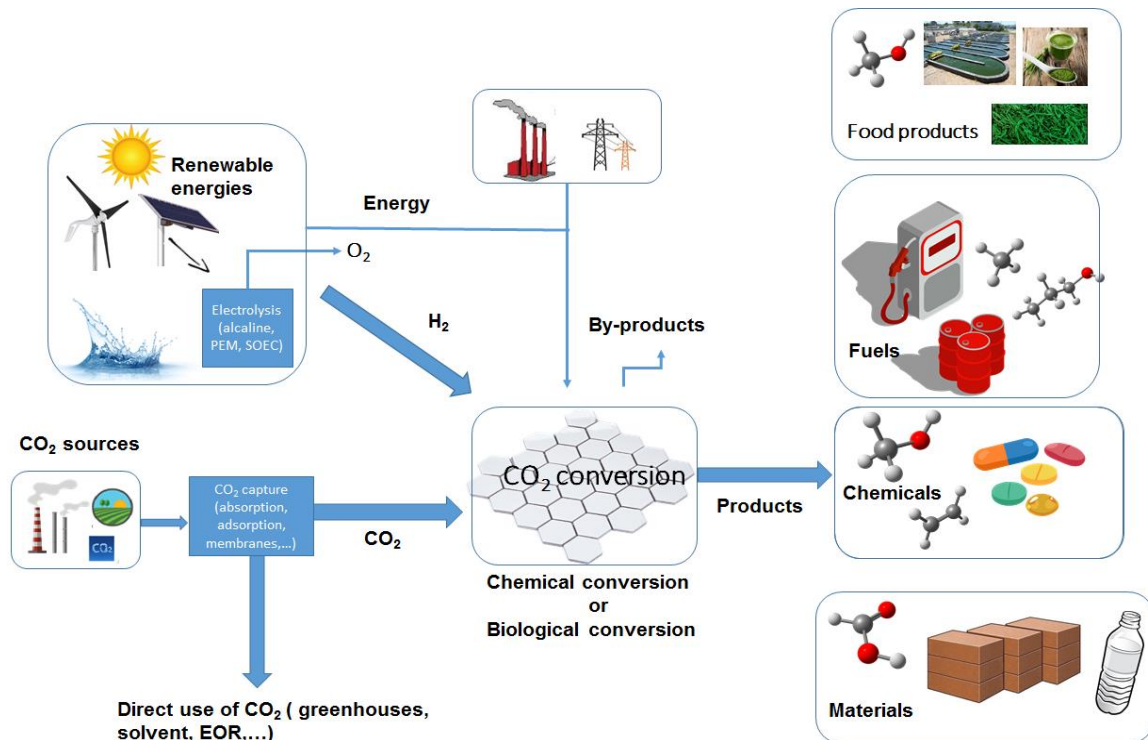


Figure 3: Example of key product chain

⁵ "Putting CO₂ to Use - Creating Value from Emissions", IEA, September 2019

The path leading from CO₂ to a given product can be direct (e.g. electrochemical conversion of CO₂) or indirect (e.g., syngas followed by thermo-chemical conversion), and based on processes of varying efficiency (in technical, environmental or economic terms). All chemical products containing carbon could in principle be synthesized from CO₂. The main barrier is the energy required to transform CO₂, a very stable molecule, into an energy carrier (as methane). The other route, functionalisation of CO₂ may require less energy but require the presence of a co-reactant that has higher intrinsic chemical energy (i.e. less negative Gibbs free energy) to enable the conversion of CO₂ at mild conditions⁶. Examples of co-reactants are epoxies and methane. Products in this category include carboxylates, carbamates, ureas and carbonates.

3.3 Sources of CO₂

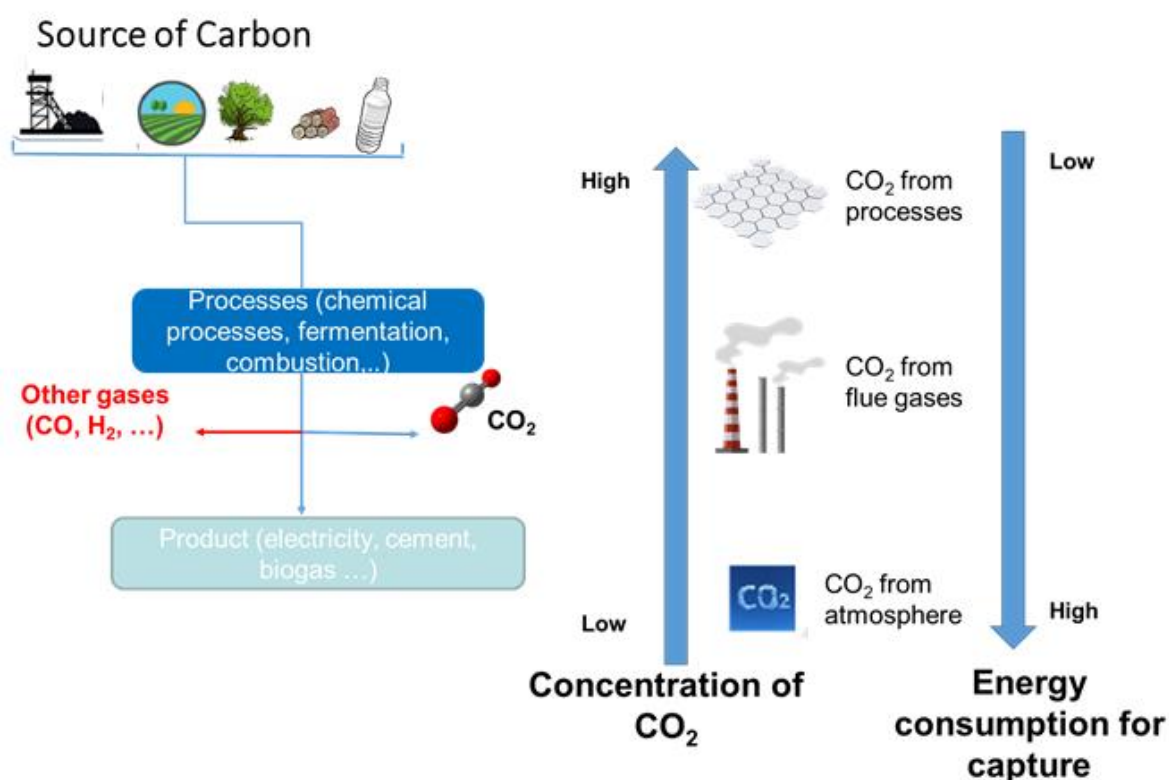


Figure 4: CO₂ sources: from concentrated to diluted CO₂

For CCU, the best CO₂ sources are those where CO₂ is available at high concentrations because of the lower energy penalty of capture. The lower the concentration of CO₂, the higher the amount of energy needed for its capture. Several LCA studies have shown that not all CO₂ sources are equivalent and the origin of the CO₂ therefore influences the results. Table 1 illustrates the wide variety of CO₂ sources from industrial processes or combustion. Because of this, the characteristics of the carbon source **shall** be described within an LCA by the CO₂ concentration, the concentration of other gases and compounds, pressure, temperature and any other specific relevant parameters.

CO₂ can also be captured from processes using biomass for anaerobic digestion, fermentation (as production of bioethanol), or gasification. In this case, even if the origin of CO₂ is biogenic, the environmental footprint of the capture **shall** be taken into account.

⁶ *Angew. Chem. Int.*, pp. 187–190, 2012

Table 1: Potential sources of CO₂ with average cost of capture⁷

CO ₂ emitting source	Global emissions (Mt CO ₂ /year)	CO ₂ content (vol%)	Estimated capture rate (%)	Capturable emissions (Mt CO ₂ /year)	Benchmark capture cost (€ 2014/t CO ₂) [rank]	Groups of emitters
Coal to power	9031	12–15	85	7676	34	Fossil-based power generation
Natural gas to power	2288	3–10	85	1944	63	Fossil-based power generation
Cement production	2000	14–33	85	1700	68	Industry large emitters
Iron and steel production	1000	15	50	500	40	Industry large emitters
Bioenergy	73	3–8	90	66	26	High purity/power generation
Hydrogen production	54	70–90	85	46	30	Industry high purity
Fermentation of biomass	18	100	100	18	10	Industry high purity

Note: estimated capture rate (%) refers here to the share of the total emissions of the full plant that will be captured by the capture unit

Recently, new developments of capture technologies have demonstrated the ability to capture CO₂ from the atmosphere. This is known as Direct Air Capture (DAC). As these technologies are at early stage, the energy required for these processes (and the costs of capture) is considerable with current capture cost estimates in the order of \$300-600/t CO₂, and estimates for future Nth-of-a-kind costs in the range of \$60-250/t CO₂⁸. As the current energy consumption of these systems is considerable, they need to be operated with renewable electricity and/or heat in order to avoid net CO₂ emissions, i.e. more CO₂ being emitted than captured.

⁷ Naims, H. Environ Sci Pollut Res (2016)

⁸ ICEF 2018. Direct air capture of carbon dioxide. ICEF roadmap 2018

4 ISO alignment

An LCA for a CCU product **shall** include the four phases of LCA (Figure 5). General LCA requirements and guidelines are provided in EN ISO 14044:2006. Regarding LCA for CCU, the following areas of special attention are covered in this document:

1. Consideration of co-products
2. Ensuring no double accounting
3. Correct attribution of impacts
4. Awareness of differences between CCU and non-CCU products
5. Origin and source of CO₂ and the products derived from this

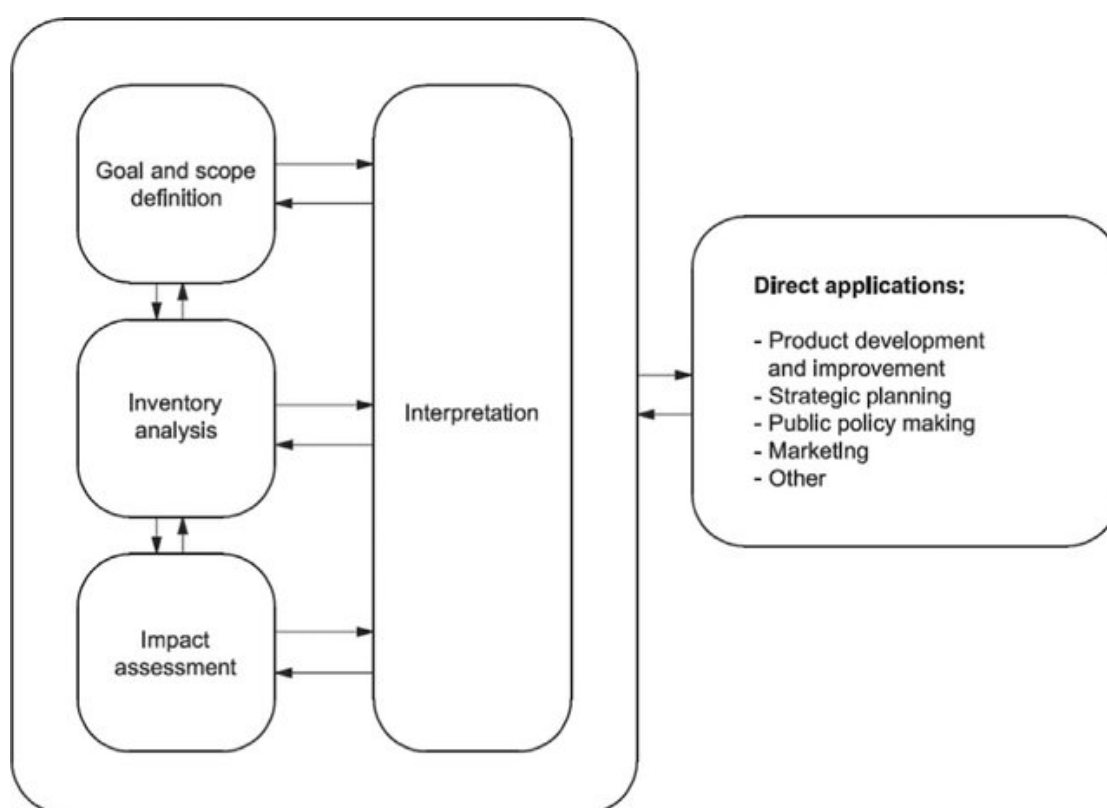


Figure 5: The four phases of LCA⁹

4.1 Goal and scope definition

The goal and scope definition is the first phase of any life cycle assessment. The goal defines the purpose of the study, i.e. the research question(s) to be answered, whereas the scope definition describes in detail the object of the LCA study, i.e. the exact product or other system(s) to be analysed.

According to EN ISO 14040 (chapter 5.2.1), the goal states a number of items such as the intended application or the intended audience. Furthermore, *“the scope should be sufficiently well defined to ensure that the breadth, depth and detail of the study are compatible and sufficient to address the stated goal.”*

For further general requirements (for *any* LCA study), we refer to chapters 6.2 and 7.2 of this report as

⁹ ISO 14040

well as to the ILCD Handbook (chapter 7).

Specific requirements for LCA for CCU studies are dealt with in chapters 6.3 and 7.3 of this report.

4.2 Life Cycle Inventory analysis (LCI)

The inventory analysis (LCI) is the second phase of any life cycle assessment. During this phase, the actual data collection, modelling of the system (e.g. product) and resultant calculations are done. This **should** be done in line with the goal definition and meeting the requirements derived in the scope definition phase.

According to EN ISO 14040 (chapter 5.3.1), the inventory analysis involves *“data collection and calculation procedures to quantify relevant inputs and outputs of a product system.”* This includes:

- Data collection,
- Data calculation, and
- Allocation of flows and releases.

For further general requirements (for *any* LCA study), we also refer to the ILCD Handbook (chapter 7).

Specific requirements for LCA studies for CCU are dealt with in chapters 10 and 11 of this report:

- Overarching data and model aspects are covered in chapter 10, and
- Selected feedstock- and energy-related aspects are covered in chapter 11.

4.3 Life Cycle Impact Assessment (LCIA)

The impact assessment (LCIA) is the third phase of any life cycle assessment. It aims at evaluating the significance of potential environmental impacts using the LCI results.

According to EN ISO 14040 (chapter 5.4.1), the inventory analysis involves *“associating inventory data with specific environmental impact categories and category indicators, thereby attempting to understand these impacts.”* The LCIA consists of mandatory elements (selection of impact categories, classification and characterisation) and optional elements (normalisation, grouping, weighting).

For further general requirements (for *any* LCA study), we also refer to the ILCD Handbook (chapter 8).

Specific requirements for LCA studies for CCU regarding the selection of impact categories are treated in chapter 12 of this report.

4.4 Life Cycle interpretation

The interpretation is the fourth and last phase of any life cycle assessment. Here, the findings from the inventory analysis and the impact assessment are appraised in order to answer questions posed in the goal definition.

According to EN ISO 14040 (chapter 5.5), the interpretation *“should deliver results that are consistent with the defined goal and scope and which reach conclusions, explain limitations and provide recommendations”*.

For further general requirements (for *any* LCA study), we also refer to the ILCD Handbook (chapter 9).

Specific requirements for LCA studies for CCU regarding uncertainty analysis are treated in chapter 13 of this report.

5 Goal definition

The goal (and scope) definition is the first phase of any life cycle assessment. It defines the purpose and the target audience of the study.

5.1 Goal of the LCA study

According to EN ISO 14044:2006 (chapter 4.2.1), *“the goal [...] of an LCA shall be clearly defined and shall be consistent with the intended application.”* Essentially, the goal definition describes the research question to be answered. The goal definition is decisive for all the other phases of the LCA. A clear, initial goal definition is hence essential for a correct later interpretation of the results.

5.2 General requirements (for any LCA study)

Although the objective of this report is to address the specificities of LCA for CCU, in this section some general requirements related to the goal definition are described, mainly for the reader’s convenience and reminder.

When defining the goal of the LCA study, the requirements of EN ISO 14040:2006 (chapter 5.2.1.1) and EN ISO 14044:2006 (chapter 4.2.2) **shall** apply.

In defining the goal of an LCA, the following items **shall** be unambiguously stated according to EN ISO 14044:2006 (chapter 4.2.2):

1. the intended application of the study;
2. the reasons for carrying out the study (and decision-context; see ILCD Handbook, chapter 5.3);
3. the intended audience, i.e. to whom the results of the study are intended to be communicated; and
4. whether the results are intended to be used in comparative assertions intended to be disclosed to the public.

In addition to these four items, two further items **shall** be identified according to the ILCD Handbook:

5. the limitations of the study: specific limitations of the usability of the LCA results due to the applied methodology, assumptions made or limited impact-coverage **shall** be identified and prominently reported (ILCD Handbook, chapter 5.2.2)
6. the commissioner of the study and other influential actors (ILCD Handbook, chapter 5.2.6).

5.3 Specific requirements for LCA for CCU studies

The proper identification of the so-called decision-context is absolutely crucial for LCA, since it directly determines a number of key aspects in all four phases of the LCA. Therefore, the formal approach to derive the applicable goal situation from the intended application and general decision-context as detailed in the ILCD Handbook (chapter 5.3) **shall** be followed.

Three different decision-context situations of practical relevance in LCA can be differentiated in Table 2:

Table 2: Combination of two main aspects of the decision-context: decision orientation and kind of consequences in the background system or other systems. Source: ILCD Handbook

Decision support?	Kind of process-changes in background system / other systems	
	None or small-scale	Large-scale
Yes	Situation A "Micro-level decision support"	Situation B "Meso / macro-level decision support"
No	Situation C "Accounting"	

Two examples of these situations are:

1. What is the macroeconomic effect for GHG reduction if the CCU system is established?
 → Meso-/macro-level decision support (Situation B)
2. What is the carbon footprint of the targeted intermediate or product?
 → Micro-level decision support (Situation A) or Accounting (Situation C)

The decision-context of an LCA study for CCU **shall** be classified as belonging to any of these three archetypal goal situations. These guidelines are intended to cover decision support situations (i.e., situations A or B in Figure 6), therefore accounting as indicated within the ILCD Handbook (situation C) is currently out of scope of the guidelines, as illustrated in Figure 6.

This classification directly determines the LCI modelling principles (attributorial and consequential) and the related main LCI method approaches (allocation and system expansion / substitution).

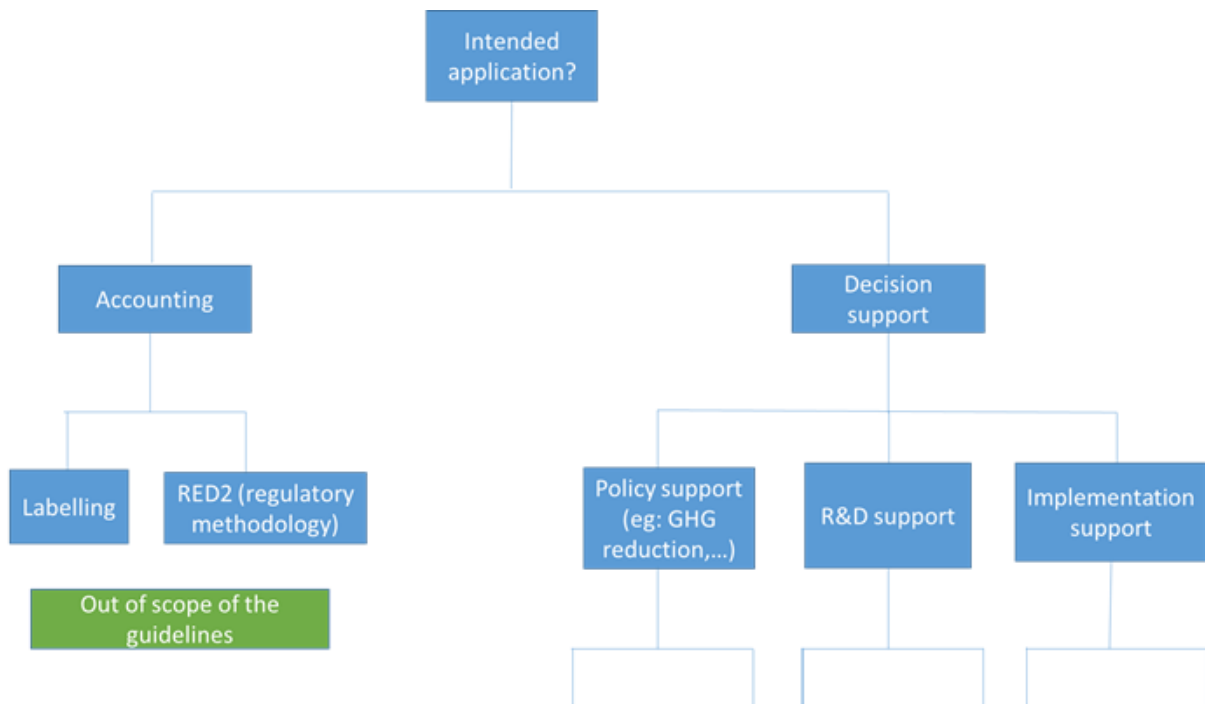


Figure 6: Decision tree to identify the goal of the LCA

5.4 Summary and key messages

The goal definition describes the research question to be answered. Since the goal definition is decisive for all the other phases of the LCA, a clear initial goal definition is essential for a correct later interpretation of the results.

In addition to the *general* requirements of EN ISO 14040:2006 and EN ISO 14044:2006, the identification of the so-called decision-context requires particular attention when performing an LCA study for CCU. The decision-context directly determines a number of key aspects in all four phases of the LCA. Therefore, the formal approach to derive the applicable goal situation from the intended application and general decision-context as detailed in the ILCD Handbook **shall** be followed.

The present guidelines are intended to cover “decision support” situations (i.e., situations A or B in Figure 6), therefore “accounting” - as indicated within the ILCD Handbook (situation C) - is out of scope of the present guidelines.

6 Scope definition

The scope definition is the second part of the first phase of any life cycle assessment. It defines what to analyse and how.

6.1 Scope of the LCA study

According to EN ISO 14044:2006 (chapter 4.2.1), *“the [...] scope of an LCA shall be clearly defined and shall be consistent with the intended application.”* Essentially, the scope definition describes the object of the LCA study (i.e. the exact product or other system(s) to be analysed) in detail. This shall be done in line with the goal definition (see chapter 4 of this report).

6.2 General requirements (for any LCA study)

Although the objective of this report is to address the specificities of LCA for CCU, in this section some general requirements related to the scope definition are described, mainly for the reader’s convenience and reminder.

According to EN ISO 14040:2006 (chapter 5.2.1.1), *“the scope of the LCA study should be sufficiently well defined to ensure that the breadth, depth and detail of the study are compatible and sufficient to address the stated goal.”* Due to the iterative nature of LCA, the scope may have to be revised due to unforeseen limitations, constraints or as a result of additional information. Such modifications, together with their justification, **shall** be documented.

In defining the scope of an LCA, all items listed in EN ISO 14044:2006 (chapter 4.2.3.1) **shall** be considered and clearly described. These include, among others, the following ones:

- Product system to be studied;
- Function(s) and functional unit
- System boundary
- Allocation procedures
- LCIA methodology and types of impacts
- Assumptions
- Limitations

Furthermore, we refer to the ILCD Handbook (chapter 6).

Product system to be studied

Based on the initial information on the process(es) or system(s) to be studied given in the goal definition, details often need to be added in the scope definition. It is recommended to provide a detailed description of the system to be studied, including technical drawings, flow charts and/or photos (adapted from ILCD Handbook, chapter 6.4). This system specification closely interrelates with the system(s)’s function(s), its functional unit(s), and its reference flow(s) which are addressed below.

Function, functional unit and reference flow

In defining the functional unit, the requirements of EN ISO 14040:2006 (chapter 5.2.2) and EN ISO 14044:2006 (chapter 4.2.3.2) **shall** apply. More details can be found in the ILCD Handbook (chapter 6.4) and in the PEF CR Guidance (version 6.3, May 2018).

The scope of an LCA **shall** clearly specify the functions (performance characteristics) of the product system

being studied. The elements of the functional unit include:

1. The function(s) / service(s) provided: “what”
2. The extent of the function / service: “how much”
3. The expected level of quality: “how well”
4. The duration / lifetime of the product: “how long”

The functional unit **shall** be consistent with the goal and scope of the study. One of the primary purposes of a functional unit is to provide a reference to which the input and output data are related. Therefore the functional unit **shall** be clearly defined and measurable.

An appropriate reference flow **shall** be determined in relation to the functional unit. The quantitative input and output data collected in support of the analysis **shall** be calculated in relation to this flow.

System boundaries

In defining the system boundary, the requirements of EN ISO 14040:2006 (chapter 5.2.3) and EN ISO 14044:2006 (chapter 4.2.3.3) **shall** apply.

The system boundary **shall** be explained clearly and in an unambiguous way, preferably in a technical flow chart. The exclusion of any life cycle stages **shall** be documented and explained.

Allocation procedures / Approaches for solving multifunctionality

Regarding the choice between different LCI method approaches for solving multifunctionality, we refer to the ISO hierarchy, as detailed in EN ISO 14044:2006 (chapter 4.3.4). This is especially relevant in the LCI phase, see chapter 11.2.

LCIA methodology and types of impacts

It **shall** be determined which impact categories, category indicators and characterization models are included within the LCA study. The selection of impact categories, category indicators and characterization models used in the LCIA methodology **shall** be consistent with the goal of the study and considered as described in EN ISO 14044:2006 (chapter 4.4.2.2).

6.3 Specific requirements for LCA for CCU studies

Specific requirements for LCA studies for CCU are listed under the following subchapters. In addition, the limitations, assumptions and methods to assess issues specific to CCU products **should** be explained.

6.3.1 Product system to be studied

These specific requirements are “outsourced” to chapter 8 of this report.

6.3.2 Function, functional unit and reference flow

Given the wide range of possible CCU products and their functions as well as different goal and scope definitions, it is neither useful nor possible to define a common functional unit. It is important that all functions of the product system are adequately captured, i.e. the service(s) delivered by a CCU-based product **should** be the basis for defining the functional unit.

First of all, it has to be determined whether the CCU process delivers a product (energy carrier/fuel, chemical, material) or an energy storage service or both.

For energy carriers such as transportation fuels, energy content (e.g. 1 MJ_{LHV}) has been used extensively as the functional unit, making it some sort of “de-facto standard” over time. However, using an energy service (e.g. 1 vehicle km using a specified means of transport) would be more appropriate to reflect

differences in fuel conversion efficiencies. The latter is especially important for CCU fuels whose chemical structure and composition can differ from their conventional counterparts (reference product) or for comparison to electromobility (where the energy content of the fuel doesn't make sense). Therefore, we recommend that in the case of CCU fuels for transportation, 1 vehicle km (or 1 tonne km) using a specified means of transport **should** be chosen as the functional unit – irrespective of whether their chemical structure and composition is identical to or different from the conventional counterpart.

The same considerations apply to other energy carriers used for heating/cooling. Although also here, energy content (e.g. 1 MJ_{heat}) is used very often, we recommend defining a FU related to the provided energy service, e.g. MJ *useful* heat. In the case of using energy content for industrial heat (steam), the temperature and pressure of the steam **shall** be reported.

In the case the CCU product (chemical or material) and the conventional counterpart (reference product) are chemically and mechanically identical, a mass-based functional unit (e.g. 1 kg of product) **should** be used. In the case of different chemical structure and composition, a specific functional unit **should** be defined based on equal technical performance.

In case of products with multiple uses, separate functional units (as well as conventional counterparts / reference products) **should** be defined and separate LCA calculations should be performed. Organic carbamates, for example, can be used as insecticides, chemical industry inputs and for pharmaceutical uses.

If the CCU process delivers an energy storage service, a functional unit quantifying the storage characteristics **should** be defined. If, however, the CCU process delivers an energy storage service *along* with a product, a functional unit quantifying the storage characteristics **should** be defined together with the functional unit of the product.

Last but not least, for the comparison of various CCU processes, 1 kg of CO₂ input **should** be used as the functional unit. All emission losses through incomplete conversion and through reactions **shall** be accounted for, to illustrate various CO₂ conversion losses.

The following Table 3 summarises the recommended functional units.

Table 3: Recommended functional units (FUs)

	Recommended FU
Product: Energy carrier - Transportation fuel	1 vehicle km (or 1 tonne km) using a specified means of transport
Product: Energy carrier - Other	Define FU quantifying the energy service
Product: Chemical/material - chemically identical	1 kg of product
Product: Chemical/material - chemically different	Define FU based on equal technical performance
Energy storage system	Define FU quantifying the storage characteristics
Comparison of various CCU processes	1 kg of CO ₂ input

6.3.3 System boundaries

Cradle-to-grave **should** be the default system boundary to assess the environmental impact of a CCU technology (see Figure 7). This means that any technical input to establish and manage the system producing CO₂ **should** be considered within the system boundary and thus be part of the LCA of the CCU product. Likewise, the use phase and end-of-life treatment (which ultimately re-releases the CO₂) **should**

be considered within the system boundary. Another key parameter is energy and that specific impacts of energy used **shall** be calculated instead of using average values (e.g., land use from additional renewable power generation and additional transmission grid capacity needed (if this is the case)). Only in this way, meaningful conclusions regarding carbon neutrality / negativity can be drawn in an unrestricted form.

However, other systems boundaries **may** be chosen, but in this case, justification **shall** be provided. An obvious exception is CO₂ obtained by direct air capture (DAC): in this case, it is not necessary to consider the primary CO₂ emitter (see Figure 8). Here, a gate-to-grave system boundary is recommended which includes the CO₂ capture process.

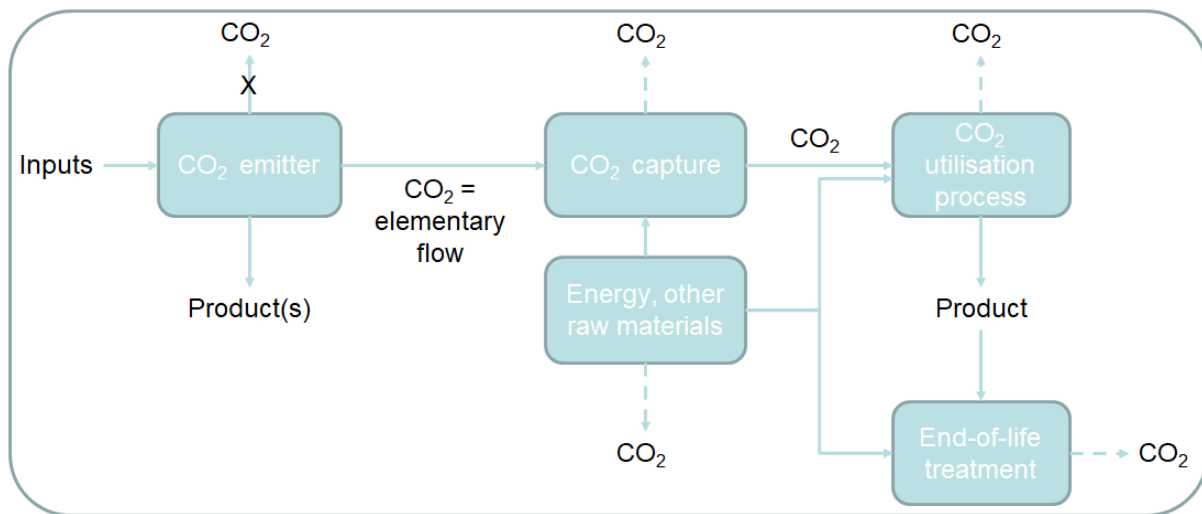


Figure 7: System boundary for fossil and biogenic CO₂: cradle-to-grave

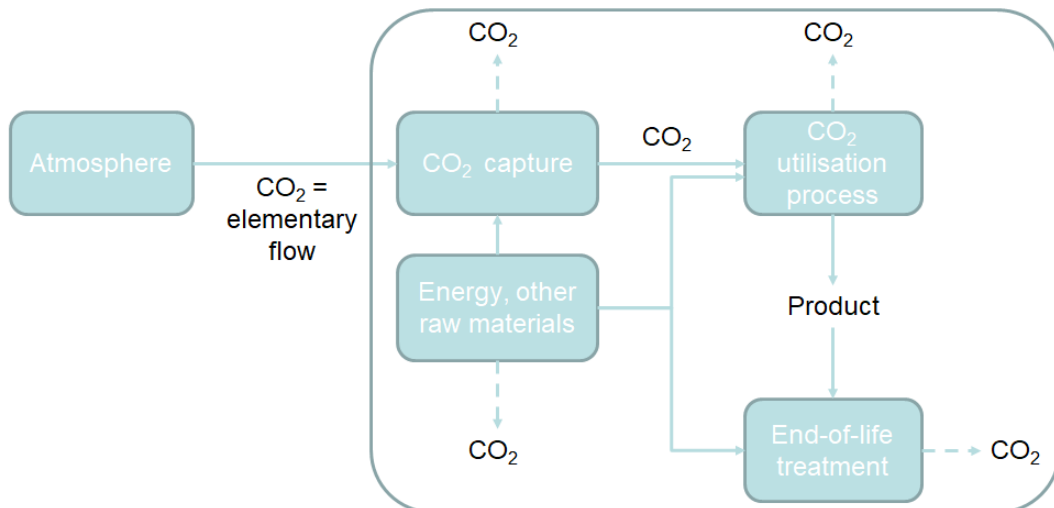


Figure 8: System boundary for CO₂ from direct air capture (DAC): gate-to-grave

We discourage the use of a cradle-to-gate system boundary, even for products (energy carriers/fuels, chemicals, materials) with identical chemical structure and composition. The reason is that the CCU product might not just substitute today's average application of its conventional counterpart but a very specific application of this chemical intermediate. A typical example is the production of a CO₂-based chemical (e.g., formic acid) which will aim to have a different application (i.e. service) in the future and therefore will have different end-of-life emissions than today (e.g., in the case of formic acid if in the

future it is intended to be used as a hydrogen carrier or a chemical intermediate instead of today's use as a preservative and antibacterial). Also, in the case of transportation fuels, non-CO₂ emissions from fuel combustion (e.g. particulate matter, SO₂ and NO_x) might differ quite considerably between CCU fuels and conventional fuels such as fossil gasoline or diesel.

The use of a gate-to-gate system boundary is strongly discouraged for three reasons:

1. The assumption that identical chemical structure equals identical downstream emissions (and therefore in a comparative study one could omit those) is only valid if the two products provide identical services. In many CCU cases, chemical compounds are intended to be produced from CO₂ for different services than today's (e.g., as energy carriers, new chemical building blocks, etc). In such cases, disregarding changes in the services and in the end-of-life emissions will result in wrong conclusions.
2. Carbon neutrality and or negativity can only be claimed if the CO₂ emissions in the upstream, the use phase and end of life are correctly considered. For a detailed discussion on this please see Tanzer & Ramirez.¹⁰
3. There is currently no standardised easily accessible LCI data on "CO₂" and more specifically on CO₂ capture technologies, thus there is no standardised data which would enable the upstream impacts to be calculated through a standard database such as Ecoinvent.

6.3.4 Allocation procedures / Approaches for solving multifunctionality

Regarding the choice between different LCI method approaches for solving multifunctionality, we refer to the ISO hierarchy, as detailed in EN ISO 14044:2006 (chapter 4.3.4). The choice of LCI method approach depends on the goal of the LCA for CCU study. Although the ISO hierarchy aims at avoiding allocation wherever possible (and to apply a system expansion approach), there are indeed certain circumstances which require determination of one product's environmental performance. In this case, a basket-of-products approach, which is for example highly recommendable for policy information at systems comparison level, is not helpful. In such cases, allocation can be appropriate and **shall** be justified. Moreover, the CO₂ burden needs to be divided between the primary CO₂ emitter and the CCU plant. This topic is addressed in detail in chapter 11.2.

6.3.5 LCIA methodology and types of impacts

Specific requirements are treated in chapter 12 of this report.

6.4 Summary and key messages

The scope definition defines what to analyse and how. In addition to the *general* requirements of EN ISO 14040:2006 and EN ISO 14044:2006, a number of *specific* requirements for LCA studies for CCU are formulated. These are mainly related to functional unit and system boundaries.

As regards the functional unit, we conclude that - given the wide range of possible CCU products and their functions as well as different goal and scope definitions - it is neither useful nor possible to define one common functional unit for LCA studies for CCU. It is important that all functions of the product system are adequately captured, i.e. the service(s) delivered by a CCU-based product **should** be the basis for defining the functional unit. It has to be determined whether the CCU process delivers a product (energy

¹⁰ Tanzer S., Ramirez A (2019). When are negative emissions negative emissions? Energy and Environmental Science, DOI: 10.1039/c8ee03338b

carrier/fuel, chemical, material) or an energy storage service or both. Based on this, we recommend functional units for a number of cases (see Table 3).

Regarding the system boundary, the present guidelines require that “cradle-to-grave” **should** be the default system boundary to assess the environmental impact of a CCU technology. Only in this way, meaningful conclusions regarding carbon neutrality / negativity can be drawn in an unrestricted form. Other system boundaries are discouraged (“cradle-to-gate”) or even strongly discouraged (“gate-to-gate”), however, they **may** be chosen on the condition that a justification is provided. An obvious exception from the “cradle-to-grave” rule is CO₂ obtained by direct air capture (DAC): in this case, a “gate-to-grave” system boundary is recommended which includes the CO₂ capture process.

In the present guidelines, further important elements of the scope definition are “outsourced” to other chapters, e.g. the description of the product system to be studied (chapter 8), allocation procedures (chapter 11.2) and LCIA methodology and types of impacts (chapter 12). The reader is referred to those chapters as well.

7 Description of CCU system

7.1 Introduction

In the scope definition, there are general requirements for any LCA.

The requirements of EN ISO 14040:2006, 5.2.1.2, 5.2.2, 5.2.3, 5.2.4 and EN ISO 14044:2006, 4.2.3 **shall** apply.

In defining the scope of an LCA, all items listed in EN ISO 14044:2006 (chapter 4.2.3.1) **shall** be considered and clearly described. See chapter 7.2.

This chapter gives CCU-specific recommendations for the description of a product system to be studied with the following aspects:

- Main processes of CCU systems: what is the product?
- Key information and parameters of the main processes
- CO₂ sources
- Carbon flows to/from the atmosphere and CO₂ pool in the atmosphere
- Comparison to the reference system
- Summary - key messages

7.2 Main Processes

The CCU system **shall** be described, covering the following six main processes in the whole life cycle as shown in Figure 9:

1. Source of CO₂
2. CO₂ capture and, when needed, compression
3. CO₂ purification and transport when needed
4. CO₂ conversion process (incl. demand and source of electricity/hydrogen as auxiliary material/energy input)
5. H₂ production
6. Distribution of products
7. Use and application of products
8. End of life/Recycling

If the “CO₂ capture” and the “CO₂ conversion process” are at the same place, they might be summarized as “CCU plant”. Ideally, they **should** not be combined so that the contribution of the CO₂ capture process can be reported separately in the assessment results (allowing for the comparison against direct air capture or other CO₂ sources)

The “CO₂ source” describes where the carbon or CO₂ is taken from and whether it is from biogenic, fossil or atmospheric origin.

The “CO₂ capture” describes the technology that is used to capture the CO₂ from the CO₂ source to make it available for the CCU system at the required specifications. If the capture unit produces CO₂ at general specifications (for instance, those required for CO₂ transport only) and the specifications are different from those required for the CCU unit, additional purification units should be explicitly specified. The units can be allocated to either the CO₂ capture or to the CO₂ conversion processes depending on the location where the purification takes place.

The “CO₂ conversion process” describes the technology that is used to produce the products from the carbon obtained by using energy e.g. electricity or hydrogen. It should contain all units required to

produce the required product specifications for the market envisioned.

The “Distribution of products” describes how the products are distributed to the place where they are used.

The “Use and application of products” describes the use or application of the products and the service that is provided by them e.g. transportation, packaging.

The “End of life/Recycling” describes what happens with the products after their use or application, e.g. recycling to new products or use for energy generation.

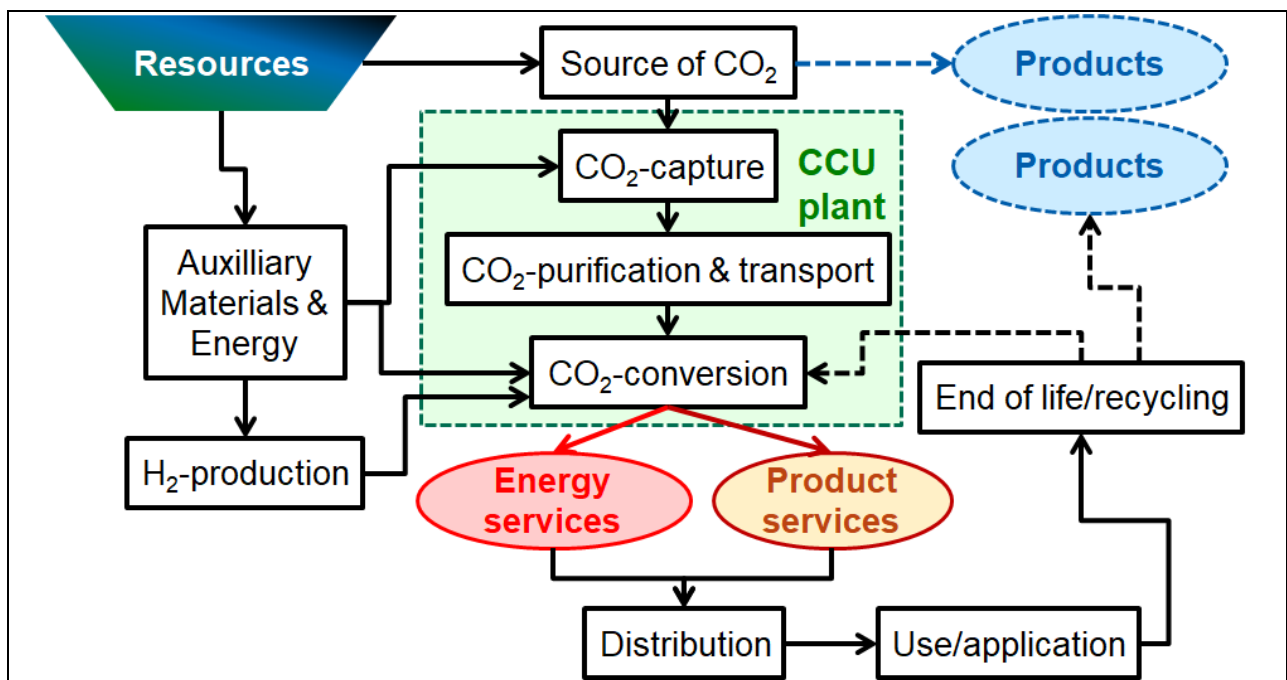


Figure 9: Main processes of the CCU system

7.3 Key information and parameters of main processes

The following specification for each of these main processes **shall** be described in detail:

1. Products: main characteristics, use/application, possible co-products
2. Current and expected state of Technology (TRL 1- 9)
3. Location/country
4. Time: today/future
5. Scale of system: e.g. as t/h, t/a, MW, TWh/a
6. Technical characteristics: full load hours, optionally characteristics of dynamic operation, efficiencies, aux. energy and material demand, direct emissions/losses of CO₂, emissions of other substances to air and water, wastes, etc.
7. Scheme of mass and energy flows between different processes
8. Quantified annual Mass and Energy balance incl. CO₂ balance
9. Various other details: e.g. pure CO₂ use in research project

For these main processes, the technical data describing the mass and energy balance **shall** be documented. The mass and energy balance **should** be on an annual basis giving also the full load hours. If intermittent electricity/energy sources are used (e.g. wind or solar) an hourly resolution over the whole

year **shall** be provided showing how the electricity demand matches with the demand of the CCU system based on real data or modelled operation characteristics. If intermittent electricity/energy sources are used (e.g. wind or solar) characteristics of the load profile of the CCU plant shall be explained in such a way and level of detail that the claimed full load hours are comprehensible (e.g., x hours at 100 % load, y hours at 50 % load, z hours at 0 % load, including for example in addition number and dynamics of load changes). In addition, mass and energy balance shall be provided for at least the main reference loads (e.g., 100 %, 50 % and 0 %). Lastly, it **shall** be described which real volatile electricity generation or provision profile the claimed operation of the CCU plant is related to.

So, in the inventory analyses the

- inputs of mass and energy and
- outputs of products and residues

shall be given for each of the 6 main processes of the CCU system.

It is important to note that the energy and mass balances change if the CCU plant is operated not at constant load but for example along with power rate provided by a volatile source such as wind or solar power. Various options for flexible operation exist (e.g., load adjustment of single units or of the whole CCU plant, change in heat integration such as partial or no heat integration, intermediate storage of electricity and/or feedstock, intermediates, products). If a CCU system is designed and operated flexibly in along with the available fluctuating electricity, this **shall** be described. If a system is to be operated flexibly, it needs to be visible in the design and data selection. An example is given in Figure 10. The example illustrates two CCU designs for the direct electrochemical conversion of CO₂ to ethylene. One of the designs operates at full load and one is designed to follow an intermittent load. In the latter case, two design options are possible, building storage capacity as part of the design (not in the figure) or designing the system in a flexible way that allows for ramping up and down. An example of such a design is shown in Figure 10, where the flexibility is obtained at the expense of heat integration. In other words, heat integration is decreased in order to allow a more flexible system. The energy and mass profiles of both systems are therefore different and will affect the LCI.

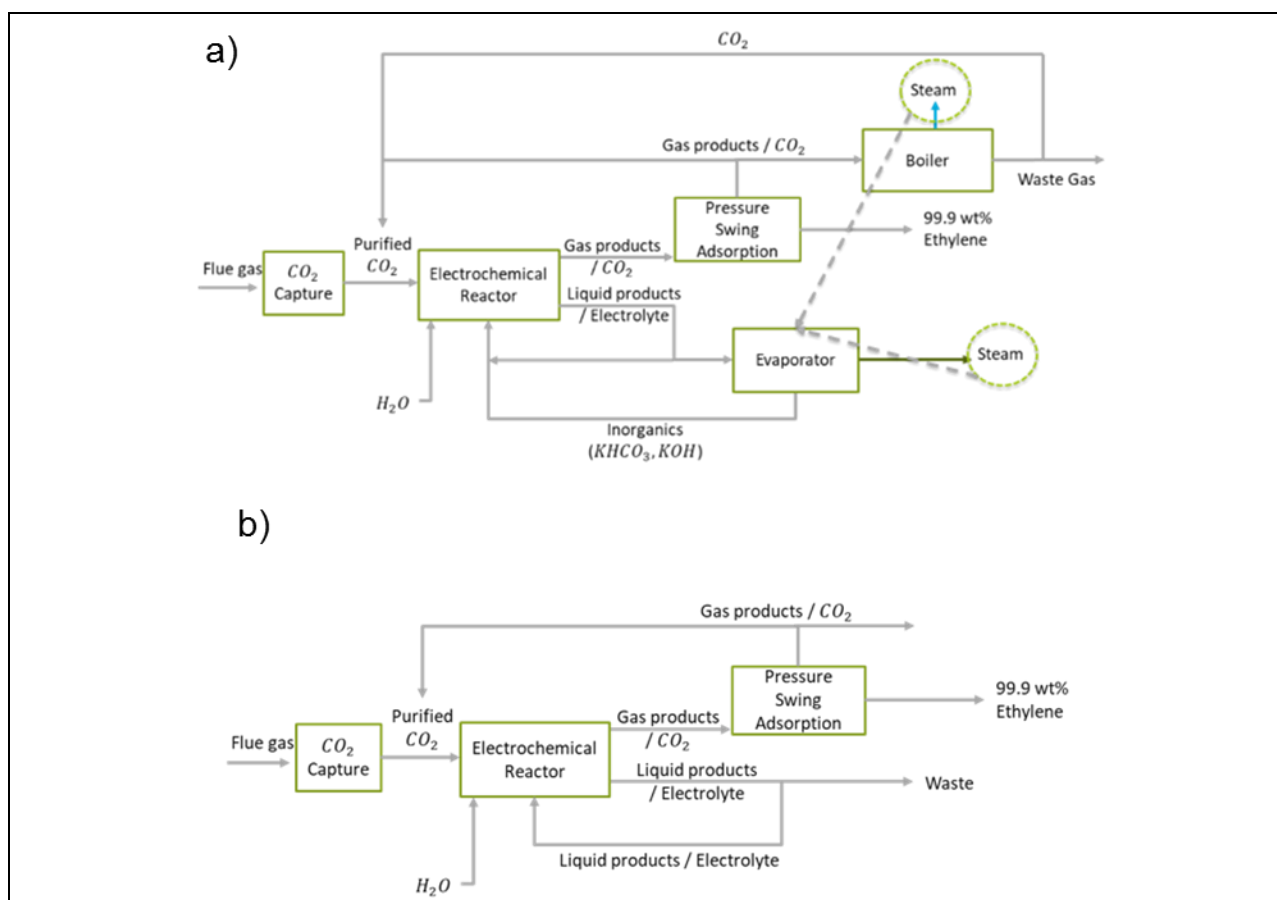


Figure 10: Example for continuous and flexible operation: Electrochemical conversion of CO₂ to ethylene a) continuous (from grid); b) intermittent from dedicated wind power¹¹

7.4 CO₂ sources

Most important is the source of carbon dioxide. The following options exist:

- CO₂ from combustion (fossil, biogenic, waste¹²)
- CO₂ from gasification (fossil, biogenic, waste)
- CO₂ from fermentation (alcohol fermentation: ethanol; anaerobic digestion: biogas)
- CO₂ from biogas upgrading to biomethane
- CO₂ from chemical processes (steel, cement, etc.)
- CO₂ from the atmosphere
- CO₂ from coal & oil & gas extraction, e.g. flaring of exhaust gases, CO₂ as a by-product of oil/gas extraction
- CO₂ from any other source, e.g. geothermal energy use

For a CCU system, the most attractive CO₂ sources (from an economic point of view) are the concentrated ones, this is because the energy consumption for the capture and purification of these concentrated sources are lower than the capture of CO₂ from diluted flue gases or from the atmosphere.

¹¹ Ege B (2019). Electrochemical conversion of CO₂ into ethylene. Master thesis, Faculty of Applied Sciences and Faculty of Technology, Policy and Management, TU Delft.

¹² which is a mixture of fossil and biogenic carbon, which has to be specified in the system description

Other C_1 sources such as carbon monoxide (CO) could also be interesting to use and are currently attracting attention.

The most relevant characteristics of the CO_2 sources are and **shall** be described:

- CO_2 concentration: vol-%
- Temperature (T) and pressure (p)
- Concentrations of other gases, e.g. CO, H_2 , H_2O , N_2 , NO_x , SO_2
- Concentration of other relevant impurities e.g. trace metals
- Annual flow: t or Nm^3 per year

The further specification of the CO_2 source **shall** include

- Primary products/services of the origin of the CO_2 source
 - Energy carrier, e.g. steam, electricity, fuel
 - Material production, e.g. steel, cement
 - None, e.g. air
- Origin of CO_2
 - Fossil fuel
 - Biogenic/biomass
 - Waste (mixture of fossil & biogenic carbon)
 - Atmospheric

7.5 Carbon flows to/from atmosphere and CO_2 pool in atmosphere

As the effects of CCU systems on global warming are very relevant, the carbon flows and pools affected by CCU System **shall** be described. So, the CO_2 flows from and to the atmosphere related to the CCU system are relevant as well as the atmospheric CO_2 pool.

In Figure 11 the scheme of carbon flows and atmospheric CO_2 pool affected by a CCU system is shown, where the source of the additional CO_2 that is an input in the CCU system is relevant. The main aspect is the additional amount of CO_2 in the atmosphere and how much additional fossil carbon is flowing from underground into the atmospheric CO_2 pool.

Figure 12 illustrates the CO_2 in the atmosphere which is affected by different types of carbon, pools and flows. For a proper carbon balance, four different pools of carbon **shall** be considered:

1. Fossil carbon stored in fossil resources
2. Biogenic carbon stored in biogenic resources, above or below ground
3. Aquatic carbon stored in water and,
4. Atmospheric carbon stored in the atmosphere.

Between these pools carbon flows. The effect of the CCU system on these carbon flows and the change of the atmospheric pool **shall** be described in the system boundaries and the results. The carbon flows and pools are time dependent and are strongly depending on the lifetime of the products.

Depending on the technology, CCU will lock up CO_2 in the product for varying time periods, While fuels or chemicals like urea only lasts for a very short period of time before the carbon is re-released, other products such as building materials could last hundreds of years, while biodegradable plastics containing a proportion of materials from CCU may degrade over a ten-year basis. The lifetime of the products is relevant to be reflected in the interpretation of the results e.g. end of life management options and the CO_2 balance, this is covered more within Chapter [12].

In the following, two illustrative examples are given – one for a CCU system producing a material and the second for a CCU system producing a transportation fuel.

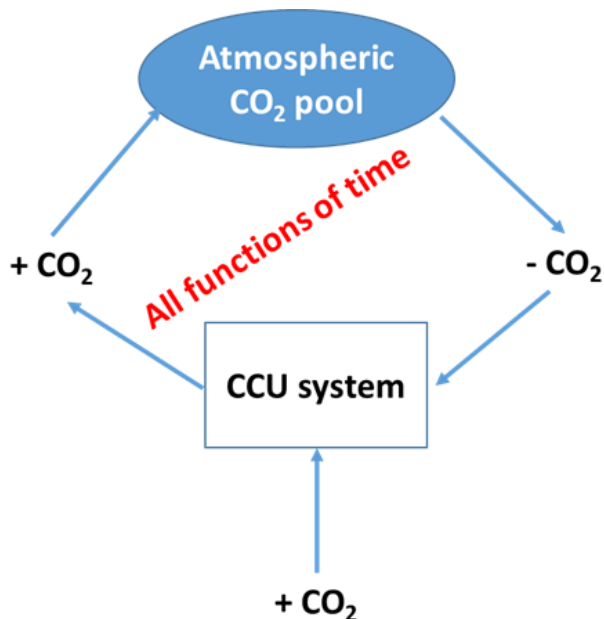


Figure 11: Scheme of Carbon flows and atmospheric CO₂ pool affected by the CCU System

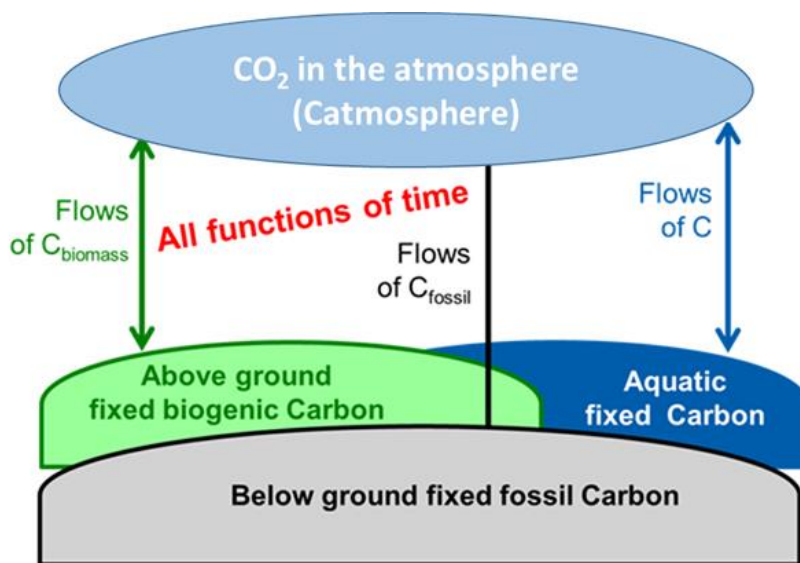


Figure 12: CO₂ in atmosphere affected by different types of Carbon, pools and flows

In Figure 13, the first example of a CCU system producing a material and its CO₂ flows is shown. CO₂ is taken from the atmosphere as a CO₂ source for the CCU system. The energy and material for the CCU system to produce the material uses (partly) fossil energy, so the supply of the auxiliaries causes a CO₂ flow to the atmosphere from fossil resources. The CCU plant fixes atmospheric CO₂ so that, in net terms, no additional CO₂ flow from the use phase occurs. At the end of life phase the material, for instance, a non-biodegradable plastic, can be landfilled, where the stored atmospheric CO₂ is fixed underground. When this is not an attractive future option, the material is combusted to produce energy and the atmospheric CO₂ in the product flows back to the atmosphere or the material is recycled to new products which in turn requires energy and raw materials. So, in total, the net effect on the CO₂ pool in the atmosphere is increased by the flow of fossil carbon from the supply of the auxiliaries over the total

lifetime of the material produced from the CCU system.

In Figure 14 a second example of a CCU System producing a fuel and its CO₂ flows is shown. CO₂ is taken from the combustion of fossil fuel, which produces an energy service, e.g. heat, for the CCU system. The energy and material for the CCU system to produce the material uses (partly) fossil energy, so the supply of the auxiliaries causes a CO₂ flow to the atmosphere from fossil resources. Then the fuel from the CCU plant - fixing the fossil CO₂ - is used to supply an energy service, e.g. transportation. As a combustion process takes place the fossil CO₂ in the product flows to the atmosphere. So, in total, the net effect on the CO₂ pool in the atmosphere is increased by the flow of fossil carbon from the supply of the auxiliaries for the CCU plant and the fossil CO₂ from the fossil resource. However, two energy services are provided, both directly by the use of fossil fuel and indirectly by the fuel produced in the CCU plant.

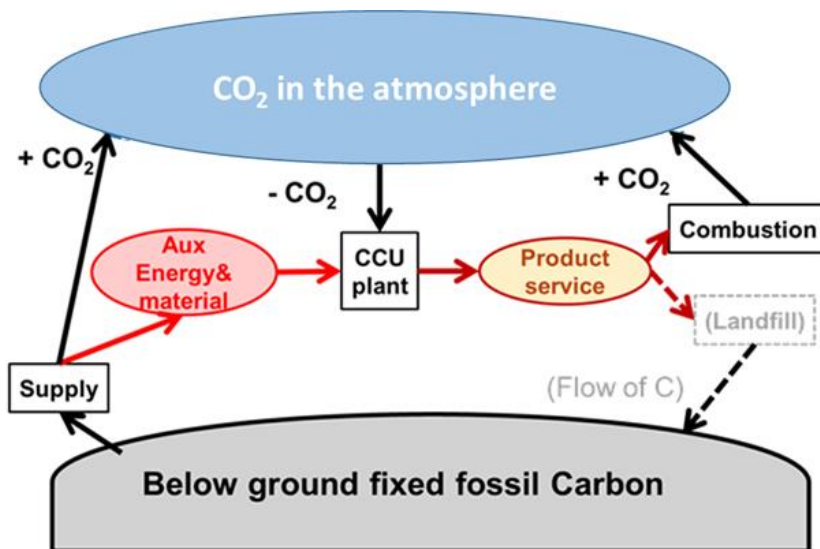


Figure 13: Example 1: CCU System (material) & CO₂ flows

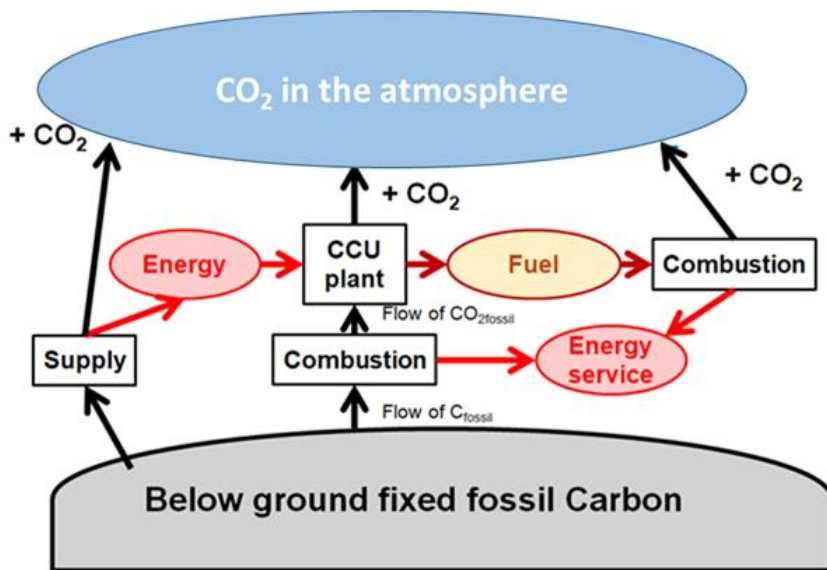


Figure 14: Example 2: CCU System (Fuel) & CO₂ flows

7.6 Comparison to reference system

The environmental effects of the products or services from the CCU system **shall** be compared to the effects of conventional or other new products and services, which is called “Reference system”. Therefore, in the comparison, the reference system and the CCU system **shall** have the same services.

The reference system **shall** be described in similar detail as the CCU system by focusing on the following issues:

- Provide same services/products
- State of Technology (TRL 1-9)
- Country/region/integration in infrastructure
- Scale/capacity e.g. kt/a
- (main) Resources (energy and mass)
- Main processes.

But beside the processes to provide the reference products and services the reference system without CCU **shall** also deal with the following topics

- Depending on the goal and scope of the LCA, relevant alternative “direct” use of renewable resources used for the CCU plant needs to be considered in the reference case: e.g. it has to be specified if additional renewable electricity is produced for the CCU plant or if renewable electricity is bought on the market or through power purchase agreements.¹³ (This is discussed in greater detail in Chapter 11).
- Current use of heating value of the C-source, e.g. current combustion of a flue gas containing CO, H₂ to generate electricity and or heat and which may not be available anymore if the flue gas is used for CCU.
- Use of “waste heat” from the reference system in the CCU system, where waste heat is defined as heat that is not used in the reference system. A more detailed discussion on this point is provided in chapter 11 of this report.
- Plausible conditions for the reference systems. For instance, unless dealing with very specific case studies, if the LCA study is conducted for the current situation, then a description of the state of technology of the reference system, e.g. Best Available Technology (BAT) for the reference system is required. If the CCU system will be deployed in the future, it should be taken into account that the reference/competing technology will also develop in the same timeline. Therefore conventional technologies may be replaced by future ones (also in the reference scenario). For example, future technologies with low CO₂ emissions, e.g. direct reduction process instead of blast furnace technology in steel making, electrolytic hydrogen instead of steam reforming or steam reforming with advanced CCS.

In the comparison, the CCU system and the reference system **shall** provide the same services, mostly energy and products, which might be supplied by the

- CCU system
- CO₂ source
- alternative use of renewable resources and
- use of the heating value of e.g. CO and H₂ from C source

¹³ The issues of alternative direct use of renewable resources will be analyzed in more detail in future work and further conclusions and recommendations will be drawn and discussed.

7.7 Summary - key messages

The key messages of the system description are summarized in the following:

- Proper description of CCU systems: products/services
- Describe main processes (e.g. TRL) and their linkages, CO₂ capture **shall** be included and described in detail
- Key information/parameters of main processes
- Special focus on CO₂ source, electricity and hydrogen (further details in chapter 11)
- Proper annual mass and energy balance, consider changes in balances in case of flexible operation
- CO₂ pool in atmosphere and CO₂ flows to/from the atmosphere from the CCU system
- Proper description of reference system with the same products/services as for the CCU system including the alternative use of renewable resources and use of the heating value of e.g. CO and H₂ from C-source

8 Data and model aspects in life cycle inventory and its related responsibilities

Life cycle assessment (LCA) is recognized as a trustworthy, scientific and understandable approach to address the environmental sustainability of human activities. It is applied for multiple uses in internal and external information supply and for decision support. However, LCA application in practice must fulfill three basic criteria: (i) It must be reliable in order to ensure the credibility of information and results generated; (ii) it must fit into existing information routines and practices in business to ensure applicability, and (iii) it must provide quantitative and relevant information to inform decision makers¹⁴.

This chapter describes the important aspects to gain reliable and realistic LCA results in the specific case of CCU. These aspects are often also generally true, but are of specific importance in the CCU case due to the relative significant scarcity of broad experience in this field.

8.1 Responsibilities

Analysing the life-cycle of well-known technologies is often complex enough and result interpretation is sometimes far from being simple. A reliable LCA result is calling for responsible practice (see¹⁵ for details). Relevant details and aspects appear partly iteratively only during the set-up and assessment of the model and sometimes certain benchmark information is available. Technologies – like CCU – with less experience, track record and scarce benchmarks are therefore even more vulnerable to unintended misleading results and need special attention and utmost responsibility of various stakeholders to ensure reliable results and the understanding of the related variations or uncertainties (as discussed in chapter 12).

Therefore, not only responsible practice, but also responsible stakeholders and cooperation is needed.

Assuming a mutual goal of getting reliable results for all stakeholders involved the need for responsible action is also evident across all stakeholders like:

- External data provider (supplier)
- Internal foreground data provider (own company)
- Method developer (mostly academia)
- Study commissioner (policy, own company, association)
- LCA background database provider (LCA database supplier)
- Study performer (institute, consultant, own company)
- Study reviewer (external expert)
- Study user (decider, influencer)

If the responsibility is taken at all relevant levels, the next step towards reliable results is an adequate LCA model.

8.2 Adequate model and data

An adequate LCA model combines realistic and complete “foreground data” (often called activity data, production/technology data or primary data) of specific nature concerning the technology under study,

¹⁴Baitz, M., Albrecht, S., Brauner, E. et al. Int J Life Cycle Assess (2013) 18: 5. <https://doi.org/10.1007/s11367-012-0476-x>

¹⁵Baitz, M. Int J Life Cycle Assess (2019) 24: 179. <https://doi.org/10.1007/s11367-018-1558-1>

with “fit for purpose” and actual background data, which covers the life cycle and supply chains around the foreground data technology (Figure 15).

Specific challenges around the CCU model set up are the scarce existing data, the immature technology level for most options and the few benchmark CCU models in LCA.

Therefore, any data source must be carefully cited. Be aware that the foreground data (quality) is highly relevant in terms of direct environmental impact (like emissions caused or saved) and indirectly as it determines use or savings of energy or alternative products.

Concerning the use of background data, its documentation must be carefully checked concerning age, technology described, fit for purpose in the given technology case, quality, consistency and completeness.

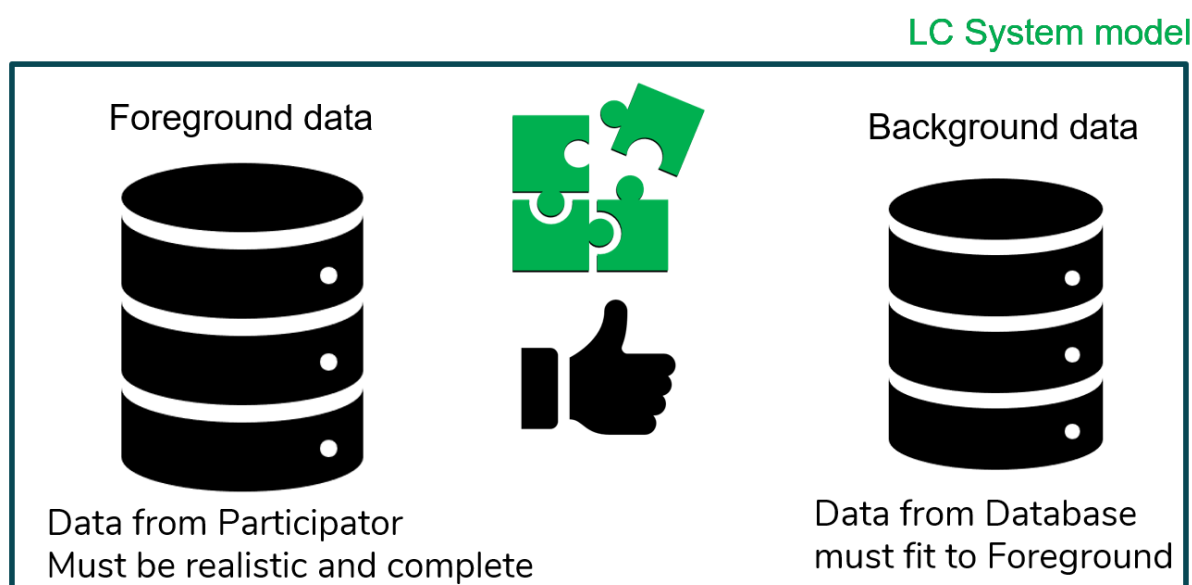


Figure 15: Life Cycle System model combining “foreground data” with “fit for purpose” and actual background data

Any LCA model – especially innovative technology models of low TRL – needs a number of assumptions to close the supply chain, the life cycle or yet unknown or undetermined aspects or possible future variations. The ISO 14040/14044 series gives humble but important guidance to deal with this issue: By interpreting the results carefully with a view on the (relevance of the) assumptions; here especially concerning CCU data gaps, own CCU technology or CCU use case assumptions and possible generic data used in this specific arena.

The origin of CO₂ could mainly influence the results of an LCA study because of the wide variety of CO₂ sources from industrial processes or combustion and the wide variety of capture technologies and energy sources that could be used. The use of “foreground data” will be the most suitable to avoid misinterpretation. In the case of the use of “background data” the most adequate data should be used. However, appropriate background data on CO₂ sources to be used in CCU is virtually not yet existing “ready to use”. Standard LCA databases provide relevant data that is needed, be the data must be adapted or specifically combined according to the specific CCU case. The responsibility to do it appropriately remains at the user’s in each case.

In practice this “interpretation of the relevance of the assumptions” is done most often either by scenario analysis in case of known and dependent technology parameters or by Monte-Carlo-Analysis in case of rather (unknown) independent parameters. Needless to say, that the latter is of less “engineering” quality.

see Chapter 13 for a more detailed discussion on uncertainties.

The used background data deserves a thorough check of the documentation, concerning

- Age
- Technology
- Quality
- Consistency

Even assuming the use of best available “representative foreground data”, adequate “representative background data” and an “adequate model” in the case of CCU, the results need to be still interpreted carefully, due to the lack of secondary impacts of CCU use cases to the “business-as-usual” case.

Specifically, representative foreground data is an issue, as own (company/technology) data is needed in the extremely specific CCU issue with virtually no benchmark existing, scarce experience, scarce average data, even more scarce public data and scarce comparability. Any study based solely on public data may hardly be able to recognize the specifics of the given CCU case, which leaves the responsibility of adequate data again to the study performer.

8.3 Overview and definition of data

LCA – not only of CCU – needs extensive data. It is not LCA as an approach, it is the reality demanding a lot of data to be reflected realistically. The life-cycle is complex and LCA is able to describe and reduce this complexity, however this is only possible with suitable data.

Any needed (background) data (pieces) may be found in LCA databases like GaBi¹⁶, ecoinvent¹⁷, and alike. As mentioned above the background data needs individual validation or treatment to adapt it to the given CCU situation, as most often no appropriate data can be directly found in databases, but is decisive for the combined result of background and foreground data. Concerning foreground data (not only but particularly), in the CCU case the core data – meaning the data describing the main activity under consideration - should be determined specifically, to make the model as realistic as possible. Even if similar core CCU data is available in a database, the chances that the related actuality, technology and geography fit to the situation under study are slim.

The core data – the data from the perspective of the CCU technology – needs to be complemented with life-cycle data towards suppliers and resources and with data towards customers, users and End-of-Life.

Core data: This kind of data originates often from processes under control or direct influence of the final producer. It is often company data of a specific situation and technology. The data is measured, calculated and/or from company systems or reports. The data reflects a specific situation at hand and influences upstream and downstream data. This core data is often also called foreground data, primary data, activity data or production data.

If the core data is not of good quality or has significant gaps the overall quality of the results cannot be good, due to the direct and indirect influence of the data on other life-cycle steps. Therefore, actuality and reality of core data is key, as it often plays the most significant role in the LCA of CCU.

Data towards supplier and resources: This kind of data originates often from processes that are maybe under control or certain influence of the final producer. It can be direct supplier data or specific secondary data reflecting specific situations. The data is measured or calculated; maybe from company systems,

¹⁶ [GaBi 2019] thinkstep AG: GaBi Software-System and Database for Life Cycle Engineering, Leinfelden-Echterdingen, Germany <http://www.gabi-software.com/international/databases/gabi-databases/>

¹⁷ [ecoinvent 2019] ecoinvent database, ecoinvent association, Zurich, Switzerland <https://www.ecoinvent.org/>

maybe secondary data reflecting the specific situation or from literature and databases. This data towards supplier and resources is often also called raw material data, supplier data or upstream data.

Data towards suppliers and resources needs to be as much as possible “fit for purpose” as CCU technologies may need very specific supply technologies. Therefore, the supplier should check the adequateness of the data (representing its supply) or the data user should check the documentation of data(set) thoroughly or may contact the data provider to ensure adequateness of the data in this case. Therefore, representativity of upstream data is key.

Data towards customer, users and End-of-Life: This kind of data originates in most cases from processes that are not under the control or influence of the final producer. Sometimes user data is available, but often this is highly variable. The data is often from statistics and most often secondary data reflecting an average situation and is derived from literature or from databases. This data towards customer, users and End-of-Life is often also called downstream data, use phase data or End-of-Life (EoL) data.

Concerning CCU data towards customer, users and End-of-Life careful assumptions are needed; especially...

- if co-product credits are involved (which may heavily influence the results by certain assumptions) or
- if use cases of CCU products are of relevant influence on the results or
- if CCU products are substituting standard products

Therefore, careful assumptions and scenarios of downstream data is key.

The different types of data are illustrated in the following picture:

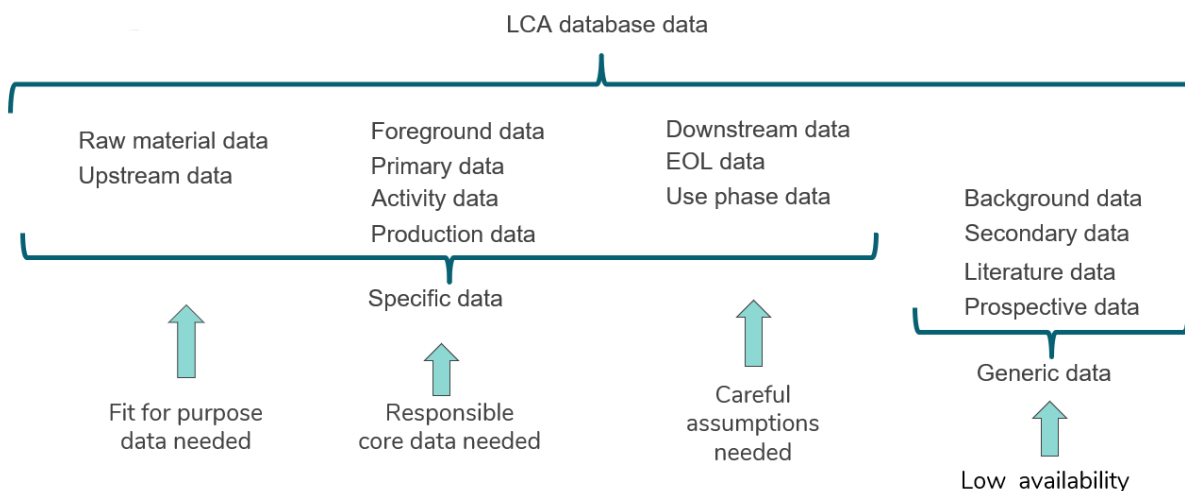


Figure 16: Types, sources and nature of different data needed in an LCA for CCU

Performing an LCA of CCU aiming realistic results calls for extraordinary attention and responsibility, because neither the study authors nor reviewers of the study can revert to benchmark results or extensive LCA publications in this field. The foundation of proper results is reliable core foreground data and adequate background data.

8.4 Potential pitfalls and sources of error in CCU

Misconceptions and mistaken investments in CCU need to be avoided. The knowledge about potential traps and possible sources of error can help to reduce the likelihood of mis-concepts and mis-investments. The most prominent aspects are listed below:

- Incomplete core data – meaning data that does not sufficiently describe the influence of the CCU technology concerning consumption of material, substances and energy as well the release of emissions and wastes - leading to cut-offs core data and in up- and downstream data.
- Use of aged, too generic, unspecific or non-representative (non-core) data.
- Misjudgement of the environmental effects of a developing technology readiness level (TRL), especially if the LCA is done in a state of a low TRL.
- Unrealistic substitution potential(s) for CCU product(s) to replace conventional products.
- Misjudgement of potential use cases and the concrete demand of a CCU product.
- Dynamic, uncertain or various potential use cases of a CCU product (e.g. methane for use as heat source or as fuel or as basis of a new synthesis route).
- Misjudgement of (secondary) effects in dynamic or partial load situations. For example, efficiencies and specific losses may vary over load. Additional energy demand may arise, e.g. for storage of CO₂s during low demands of by-products. Further the quality of feedstock and energy may vary under dynamic circumstances.
- Underestimation of impacts from building materials for CCU plants, renewable power generation and infrastructure such as for transmission grid or CO₂ pipelines.
- Difficulty to predict implications during scaling-up of lab-scale plants to industry level.
- Focus on GHG only and omission of other environmental impacts.
- Overestimation of availability of CO₂ sources and underestimation of costs to capture and provide CO₂ for conversion (or - see also above - use unspecific data for provision of CO₂).

It can be summarized that potential traps and sources of error in CCU can best (or even only) be avoided by performing sensitivity and scenario analysis on the basis of the dynamic, uncertain, missing or assumed data points.

8.5 Considerations concerning gap closing

Missing data does not necessarily lead into the neglect of data in LCA. The most obvious way to close a data gap is to search available LCA databases for processes or proxies (e.g. PEF/OEF DB¹⁸], GaBi DB , ecoinvent DB). A relevance check of the data gap **should** be performed on the basis of a rough “best case” and “worst case” assumption. It is always recommended to try different scenarios of various gaps closing options. If the relevance of the gap seems to appear small it is recommended to apply the worst case regarding the data used (as the data point influences the result anyway only to a minor extent). It is better to adjust the result later towards a slightly better result, than to be forced to communicate worse results after the data precision increased.

Avoidance of (unintended) green washing generally has a high priority. Therefore, the use of a “precautionary principle” and a rather conservative approach for gap closing is recommended.

8.6 LCA Data collection, handling and provision

To enable use of consistent LCA data and to deal with potential gaps, variabilities and assumptions in CCU data consistently and independently from particular databases or software, we recommend a

¹⁸ [EU EF 2019] The Environmental Footprint database (EF data), European Commission https://ec.europa.eu/environment/eussd/smgp/PEFCR_OEFSR_en.htm

transparent governance process for identification of gaps in existing CCU data and LCI data collection and a provision of software/database independent format (like ILCD format) for these processes.

8.7 Conclusion

Concluding this chapter, it can be summarized that three areas need to be addressed properly to gain reliable and mindful LCA results (of CCU): Data, model and responsibility (Figure 17).

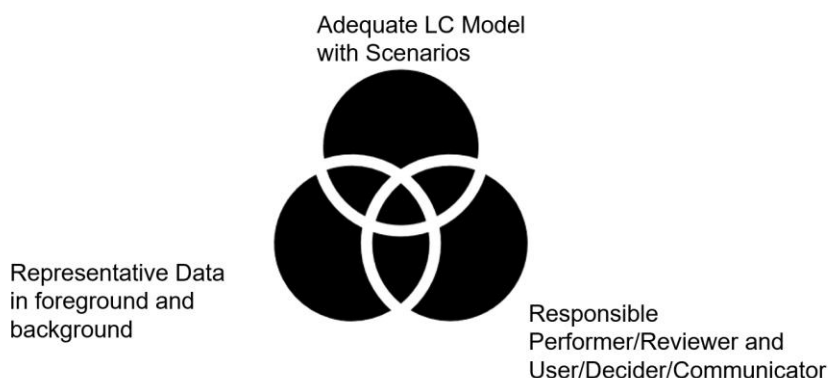


Figure 17: Three areas to gain reliable and mindful LCA results (for CCU)

A suitable LCA for CCU model should reflect the (complex) reality adequately. Oversimplification **should** be as much avoided as unnecessary complication. Data consistency and representativity needs to be ensured in foreground and background. The Life Cycle Inventory (LCI) consistency is key. This includes the use of standardized elementary flows, the avoidance of double counting as well as omissions. Life Cycle Impact Assessment (LCIA) consistency needs to be addressed via the use of adequate impact models that are able to characterize the majority of the needed flows. Sensitivity analysis and the use of parameters and scenarios at points of variable and/or uncertain technical aspects is highly recommended. Careful interpretation with regard to data gaps, dynamic aspects, assumptions and responsible communication is important.

9 Feedstock- and energy-related aspects

9.1 Introduction

Conversion or activation of CO₂ typically goes along with high specific energy demand, either by reaction with at least one energy carrying reaction partner such as hydrogen or ammonia or by direct energy input such as in high temperature co-electrolysis or plasma pyrolysis. Consequently, indirect emissions often have high relevance for the overall footprint of a CCU process. Feedstock- and energy-related emissions thus need to be very thoroughly looked at to ensure quality of LCA. Likewise, methodological differences in this area can have a high impact on overall outcome and comparability between separate studies. The following chapter provides recommendations for selected feedstock and energy carriers in LCA. The examples represent representative CCU cases and illustrate the approach of consequential life cycle modelling which is preferred in case of LCA for decision making as is the focus of this report.

9.2 Credits and burden for CO₂

By definition, CO₂ is an elementary feedstock for CCU plants. At the same time, it contributes to a fundamental impact category (global warming potential, GWP), both for its source (e.g., emitting plant) as well as the CCU plant itself. For the emitting plant, CO₂ is typically not the main product, often rather an undesired side product. Upon utilisation of the CO₂ instead of emitting it to the atmosphere, it is of relevance who gets the credit for reduction in CO₂ emission or, in other words, how to allocate the CO₂ emission reduction between emitter and receiver of CO₂. In order to avoid uncertainty or even misuse, unambiguous rules for allocation of CO₂ emissions are essential. Three schematic reference cases will be described here.

In view of the relatively long potential life-time of industrial plants as well as the relatively short remaining period left to develop a fully sustainable economy, proper selection of reference systems is generally crucial to ensure LCA results which are consistent with future developments. Details will be elaborated below along with the respective cases.

9.2.1 CCU plant is added to an existing CO₂ emitting plant without further interaction

A sort of base case is the installation of a CCU plant next to an already existing CO₂ emitting plant. Figure 18 illustrates this case. The primary emitter could for example be a fossil fuel-based power plant (product A = electricity) and the CCU plant a Methanol production plant (product B = Methanol).

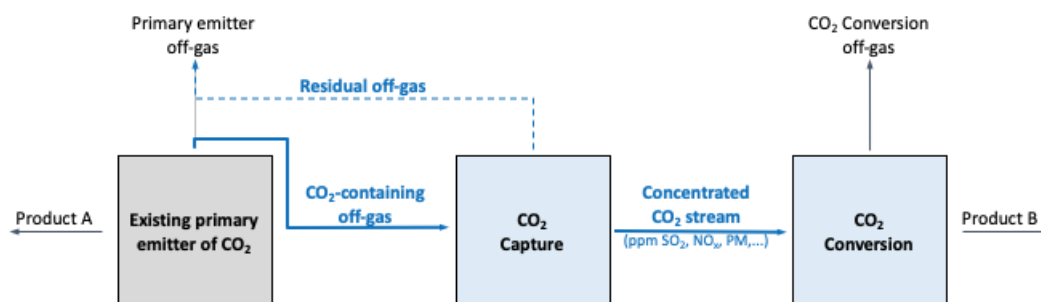


Figure 18: Schematic flow of CCU plant exploiting CO₂ from a primary emitter which, besides providing CO₂ does not change its operation

A portion or all of the CO₂ from an off-gas which was emitted so far by the primary emitter is now captured and sent to the CO₂ conversion plant where the CO₂ is converted to product B. Not-converted CO₂ leaves the CO₂ conversion plant by a (separate) off-gas. Together with CO₂ from the off-gas of the primary

emitting plant, minor amounts of other components with environmental impact such as SO₂ or NO_x may cross the system boundary to the CO₂ conversion plant. Besides the CO₂ stream, no other material or energy flow such as heat or power connects the two plants. Especially, the primary CO₂ emitting plant does not change its operation and specific consumptions and product output upon operation of the CCU plant.

According to consequential modelling, it is the merit of the CO₂ conversion plant that in total less CO₂ is emitted from the primary emitter to the environment. Thus, for any LCA applying cradle-to-grave as system boundary (such as recommended above in chapter 5.2.3.), the primary emitter **should** be treated as if no change had occurred (so-called 100:0 allocation). Consequently, reduction in CO₂ emissions **should** be allocated to the CO₂ conversion plant by respective negative GWI. All direct and indirect emissions associated with the CO₂ capture **should** be allocated to the CO₂ conversion plant, except for cases in which CO₂ needs to be separated anyway to obtain a marketable product A (e.g. ethylene oxide production, biogas upgrading to biomethane). Deviations from this rule **shall** be justified and documented. For example, other options to allocate CO₂ emitted from the primary source could be a 50:50 allocation¹⁹ or a 0:100 allocation, the latter becoming meaningful in an increasingly decarbonised economy where concentrated CO₂ would become a scarce resource and thus could be treated as a co-product.

All CO₂ entering the CO₂ conversion plant but leaving it again because it has not been converted, **should** be counted as emission of the CO₂ conversion plant, likewise, all other emissions present in the CO₂ stream entering the CO₂ conversion plant (e.g., ppm of SO₂ and NO_x).

The procedure proposed here builds on the existing primary CO₂ emitting plant as a reference system. For almost every potential source of CO₂ it is to be questioned to which extent the existing plant represents state-of-the-art in the respective area and will continue to do so in the mid- to long-term. For example, a CCU plant being installed next to a coal-fired power plant may result in stranded assets once the power plant will be shut down in the framework of generally decarbonising power generation. In order to avoid such undesirable cases - both from a micro- as well as macro-economic point of view -, the LCA **shall** include a sensitivity analysis with respect to future and especially ultimately sustainable technologies to produce the main product (product A in Figure 18). In many cases, it is not yet clear how those future technologies will look like or there are several options. This could render the sensitivity analysis demanding. Yet, due to the very high relevance, it would not be acceptable to omit the sensitivity analysis just because of uncertainty. In order to provide better guidance for practitioners in this context, it could make sense to develop reference cases for selected important areas such as in steel, cement or chemicals production (beyond the scope of this study). In addition to using reference cases for sensitivity, it is recommended to also use direct air capture (DAC) as a sensitivity scenario.

Especially in the case of LCA for low-TRL CCU technologies but also for cases where CO₂ is transported via a pipeline grid, for example connecting several CO₂ sources and users, the link of a specific CO₂ conversion plant to the source might not yet be clear at the point in time the prospective LCA is executed. In order to avoid excessive study of many possible sources the practitioner might reasonably decide to apply a gate-to-gate system boundary for LCA. In contrast to the case described above, the CO₂ **should** then be allocated to the CO₂ conversion plant (0:100 allocation). Only this way, it is made sure that the CO₂ has not been “double omitted”. If the LCA practitioner wants to apply other rules than this, he/she **shall** state the reason. Especially, he/she **shall** explain how an unambiguous allocation of CO₂ to the source and/or the CO₂ user can and will be ensured.

¹⁹ Allacker et al. 2017: The search for an appropriate end-of life formula for the purpose of the European Commission Environmental Footprint initiative; Int J Life Cycle Assess (2017) 22:1441 - 1458

9.2.2 Existing CO₂ emitting plant is operated differently after installation of CCU plant

The situation gets more complex if the primary emitter is operated differently upon combination with a CCU plant (see Figure 19 for illustration). For example, a power plant producing electricity (= product A) provides steam for the CO₂ capture process and in consequence produces less electricity. Another example is a CCU plant which receives a gas stream from a steel mill containing also hydrogen and at least some portion of this hydrogen is exploited by the CCU plant which otherwise would have been utilised for power and/or heat production.

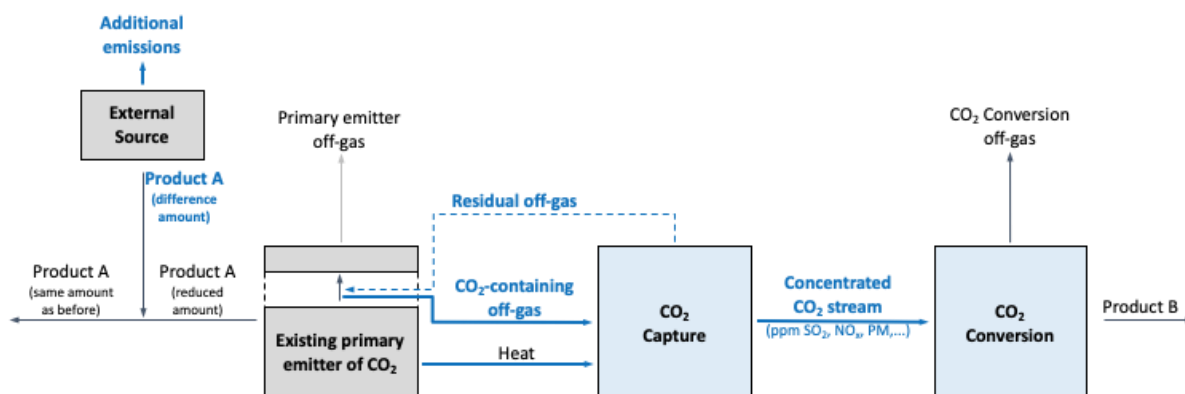


Figure 19: Schematic flow of CCU plant exploiting CO₂ from a primary emitter which, upon provision of CO₂ changes its operation

In general, this case can be treated as for the previous one (11.2.1.), i.e., it is the merit of the CO₂ conversion plant that upon operation, in total less CO₂ is emitted to the environment. So, the primary emitter **should** be treated as if no change had occurred, i.e., as if being operated as before. Again, reduction in CO₂ emissions **should** be allocated to the CCU plant by respective negative GWI. Other trace emissions being present in the stream of captured CO₂ (e.g., ppm of SO₂ and NO_x) **should** be treated as in the previous case, i.e., they **should** be allocated to the CO₂ conversion plant. Deviations from these rules **shall** be justified and documented.

The change in product output of the primary CO₂ emitter upon operation of the CCU plant though needs refinement of the rules. According to consequential modelling, all reductions in product output, e.g., reduction of electricity produced, **shall** be compensated arithmetically by corresponding system expansion and including respective additional emissions (see Figure 19). Those additional emissions occur upon installation and operation of the CCU plant and hence **should** be allocated completely to the CCU plant. In case of compensation of reduced electricity production, the guidelines of section 11.3 shall be applied accordingly (i.e., as “additional electricity” demand). Again, deviation from these general rules **shall** be justified and documented.

As in the previous case (11.2.1.), a sensitivity analysis **shall** be included in the LCA with respect to future technology developments in the area of primary CO₂ emitting plants.

Regarding LCA for low-TRL CCU technologies or for cases where CO₂ is transported via pipeline grid, as already discussed in section 11.2.1., the CO₂ **should** again be allocated to the CO₂ conversion plant (0:100 allocation). If the LCA practitioner wants to apply other rules than this, he/she **shall** state the reason. Especially he/she **shall** explain how allocation of CO₂ to the source and/or the CO₂ user can and will be ensured.

Correspondingly, in LCA for CO₂ capture from a primary emitter where the CO₂ is fed into a pipeline or for other reasons the additional emissions resulting from system expansion can not be linked to a single CO₂ user, all these additional emissions **should** be calculated and stated separately.

9.2.3 CO₂ emitting and CCU plants are built together

In case a primary CO₂ emitting plant is built together with a CCU plant, either similar to case 11.2.1 or similar to case 11.2.2, consequential modelling on the one hand does not provide clear guidance as to how to allocate CO₂ emissions. On the other hand, due to the higher likelihood that both plants may have a life-time reaching to or close to a fully sustainable world, even more care **should** be taken to adequately model both present as well as mid- to long-term impact.

Considering the diversity and uncertainty of potential technology developments for various industries, both for the ones emitting CO₂ and for those utilising it, it is hardly possible to provide concrete generic rules here. Rather, it is recommended to develop and agree industry-wise on a set of limited technology scenarios and respective rules which then **should** be applied in LCA. For example, the scenarios for steel industry could include conventional blast furnace technology using some sort of renewable coke feedstock and/or recycling mill gas in the blast furnace, alternatively, DRI using renewable synthetic methane or other gas and DRI using hydrogen. Likewise, scenarios for power production from biomass or waste could include alternative generation of power by other renewable sources such as wind and PV power plants.

As long as such scenarios are not yet available, LCA for combined new-built CO₂ emitting and utilising plants **shall** be executed according to cases 11.2.1 and 11.2.2 with the additional requirement that independent on the concrete technology to be realised, Best Available Technology (BAT) **shall** be used to represent the primary CO₂ emitting plant. The LCA **should** further include sensitivity analyses based on assumptions for the development of BAT in the future as to make sure that LCA is robust against corresponding technological progress.

9.3 Electricity for direct use within a CCU plant and/or for production of H₂

9.3.1 Preliminary remarks: Electricity - increasingly relevant but also challenging in LCA

In the long run, renewable electricity will be a central pillar of a sustainable global economy. At the same time, several uncertainties are associated with the transition to and even the ultimate setting in a world built extensively on renewable electricity. Some general remarks are thus necessary prior to concrete recommendations for adequate modelling within LCA.

Beyond substitution of fossil and nuclear power for conventional electricity applications, two main concepts exist to build on renewable electricity, i.e.,

- by electrification of processes which were operated by the use of fossil energy carriers so far (e.g., a coal- or natural-gas fired boilers) and operation on renewable electricity, or
- by production of chemical energy and energy carriers respectively from renewable electricity such as hydrogen and derived products (e.g., SNG, methanol, synthetic aviation fuel, ammonia) and by application of those carriers such as for mobility or heating.

Those two general options also may be applied to produce sustainably chemicals or other carbon containing materials from CO₂, e.g., direct electrification via co-electrolysis or plasma-splitting of CO₂ or via production of hydrogen from electricity and subsequent conversion with CO₂ to, for example, alcohols, olefins, or other chemical feedstock and products.

So, on the one hand, renewable electricity is an extremely important and versatile element of a future sustainable world and consequently will be highly relevant for LCAs. On the other hand, the special characteristics of renewables render adequate modelling within LCA very challenging. Wind and PV power have by far the highest potential for capacity expansion globally and are likely to dominate provision of electricity generation ultimately. Yet, they go along with significant volatility. It is foreseeable that even at high shares of renewable electricity there will be times when production would not cover current

demand. A CCU plant designed for operation on preferably renewable power has to consider such constraints by either assuming temporarily reduced power consumption (or even shut-down), by inclusion of some sort of electricity storage or by inclusion of at least limited operation with non-renewable power (resulting in correspondingly higher environmental impact). It is evident that plant design, temporal profile of available renewable electricity and real load profile of a CCU plant are linked to each other.

Current state-of-the-art of modelling electricity from the grid in LCA is to use data being averaged annually and across a specific mix of power production technologies. In an advanced case, electricity from the grid is refined to a residual grid mix which excludes all claimed and tracked renewable electricity. In the past, this was adequate and practical. However, in view of the above-mentioned developments and increasingly dynamic changes in boundary conditions, a more time- and even space-resolved modelling is needed including long-term impacts from capacity build-up both on the production as well as the demand side.

It is hardly possible if possible at all for a single LCA practitioner to provide such a sound and certain model of the future. On the other hand, there is a high need for such models. For example, the current controversy about whether we should pursue to an utmost extent pure electromobility or also use synthetic fuels (H₂ and derived fuels) in fact results vastly from separate models and assumptions for future build-up of renewable power capacities. It is thus highly recommended to develop solutions in the above context which then may serve as reference for LCA practitioners. One option could be to agree (at least industry-specifically) on scenarios which might then be applied by the LCA practitioner.

In the meantime, it is strongly recommended that the LCA practitioner **should** define his own scenarios and apply them within LCA. If he doesn't follow this rule the practitioner **shall** document his reasons.

Independent on those challenges, some general guidelines which will be elaborated below could help to improve LCA modelling.

As a concluding remark and in order to avoid misunderstandings, it is important to state that despite the above-mentioned challenges, LCA remains as the best tool to assess environmental impacts of technologies and to provide related information for decision makers in politics and economics. It is not the LCA but the models of the real world which need refinement to improve validity and explanatory power of LCAs.

9.3.2 Electricity from additional renewable power plants via Power Purchase Agreements (PPAs)

Due to its typically high relevance for LCA of CCU plants, electricity, either used directly or indirectly (e.g., for production of hydrogen) should have low environmental impact, especially low GWI. From a system point of view, a momentary additional electricity consumption results in the necessity to provide an equivalent additional amount of electricity. Since most of the renewable power plants typically operate at their maximum output, the additional amount of electrical energy is provided by a conventional power plant, most often a coal- or gas-fired power plant. Claiming a portion of renewable power from an already previously existing renewable power installation for the CCU plant, e.g., by certificate, would overall not change the situation. In line with consequential modelling it is thus not acceptable within LCA to allow any additional power consumers including CCU plants to claim renewable electricity from previously existing renewable power installations.

The situation is different if the renewable power installation is built along with and because of the building of an additional power consumer such as a CCU plant. In this case, renewable electricity added to the system may be attributed directly to the CCU plant. Hence, a clear and straight-forward case to claim renewable electricity for a CCU is installation of corresponding additional renewable power capacity. If this is pursued in the model of an LCA, the practitioner **shall** explain how such additionality is ensured. Besides installation on-site and physical connection, Power Purchase Agreements (PPA) may be an

adequate proof.

The same holds likewise for cases where previous power production will be reduced along with installation and operation of a CCU plant (see case 11.2.2). The additional amount of electricity to be provided from a separate source **shall** be claimed renewable only, if the respective generation plant is erected in addition.

In view of the above-mentioned potential restrictions by grid capacity, the LCA practitioner **should** further explain how it is made sure that such restrictions are not relevant for him or provide a corresponding sensitivity analysis. Deviations from those rules **shall** be justified and documented.

In case of additional wind and PV power installations, the question arises whether operation of the additional power consumer, e.g., CCU plant, needs to be operated at maximum along the momentary power production capacity or if it would be sufficient to match the produced electricity on an annual energy balance. The latter approach is highly preferential for a single operator since it would allow him to run his plant at much higher full load hours. From an LCA point of view though, this would be acceptable only if the environmental impacts from third parties' power production in times when the plant's load exceeds the renewable production are at least compensated for by the avoidance of environmental impacts in times when the renewable plant produces above the load of the CCU plant by substituting conventional power generation.

Again, this could require more or less complex modelling of systems effect. As a concrete guideline it is recommended that the LCA **should** state, whether, and if so, how the plant design and operation concept fits to the production profile of the claimed renewable power installation. Furthermore, it should be stated how timewise matching of power generation and consumption is ensured. If alternatively it is assumed that the electricity of the renewable power installation is claimed on an annual energy balance, the practitioner **shall** elaborate and document how it is made sure that the total of environmental impacts in times of over- and underproduction of renewable power are not higher than in case of operation along the production profile of the renewable power plant.

In view of potential future limitations in renewable power and/or transmission grid capacity expansion, it is - not only but especially for policy makers - of interest to get an idea of related implications of a large-scale deployment of the technology. The LCA **should** thus provide an approximation of additional renewable power production and grid capacity demand in case of large-scale technology roll-out. Again, deviations **shall** be justified and documented.

A special but increasingly relevant case arises from renewable power installations running out of feed-in tariffs. The implications for LCA may get more complex than it appears. In line with the above rules, such plants **should** first **not** count as additional renewable power. In fact, most PV installations have much longer lifetime than the period of feed-in tariffs and **should** correspondingly **not** be treated as new-built, additional renewable power. On the contrary, most of the wind power plants need at least some more or less significant maintenance or even refurbishment prior to continued operation. One could argue that those plants would be shut down and not available any more without maintenance or refurbishment. On the other hand, as also a study among German operators of wind power plants running out of feed-in tariff in the next decade shows²⁰, the related costs may differ strongly among plants and especially may be significantly lower compared to a new build. It would be adequate to claim that a significant share of the wind power plant has already been paid by society through former feed-in tariffs.

Due to the increasing relevance of the matter, it is recommended that further guidance should be provided on such cases. One option would be to compare the costs incurred by maintenance and

²⁰ (available only in german) A.-K. Wallasch et al., Perspektiven für den Weiterbetrieb von Windenergieanlagen nach 2020 (2017)

refurbishment and to compare those costs to a completely new-built power generation at the same site at the time of maintenance and refurbishment. The ratio of costs could be interpreted and dealt with as the share of capacity which was built as additional capacity.

9.3.3 Electricity from specific conventional power plants by defined contracts

Even though renewable energy will be a main driver and a main prerequisite for meaningful operation of many CCU technologies, it is also important to clarify treatment of electricity from conventional power plants within LCAs. First, there are other options besides renewables with reduced environmental impact, especially GWI, from power generation, for example nuclear power or power from clean hydrogen (e.g., produced via SMR (Steam Methane Reforming) +CCS or via pyrolysis of natural gas, see also section 11.4). Second, as already mentioned in the previous section, conventional power such as from natural-gas fired power plants will be essential for the transition period to a fully sustainable electricity system.

In case an LCA claims some sort of reduced environmental impact for electricity consumed, as for example from power plants listed above, the practitioner **should** first specify that and how this is made sure by contract. Second, in the case of nuclear power generation, it **should** further be documented how it is made sure that the power claimed will be produced in addition. This is to avoid that the corresponding electricity is just shifted from one to another application and in fact another sort of power has to be produced to cover the additional demand.

Likewise, for other specifically claimed conventional electricity such as from natural-gas fired power plants the LCA **should** document how it is made sure that the respective amount of electricity will be produced in addition upon the additional demand by the CCU plant.

As for renewable power generation, the LCA claiming some specific reduced-impact or conventional power **should** always include a statement on how it is ensured that there will be no restrictions by transmission grid capacities or provide respective sensitivity analyses. Deviations from the guidelines above **shall** be justified and documented.

9.3.4 Electricity from the grid

Even in case of unspecified electricity consumed from the grid, refinement of guidelines with respect to LCA is meaningful. As already stated, the more volatile renewable power gets into the market the more all other plants will be operated also time-dependently. It is thus more than adequate to define operation and boundary conditions of all electricity providers including conventional ones also time-dependently, i.e., to use for example hourly-resolved instead of annually averaged data.

Since, as also already stated, an additional demand of electricity, e.g., by a CCU plant, will require a corresponding additional amount of electricity to be produced, e.g., a gas-fired power plant, it would be expedient to attribute the environmental impact of the respective additional unit of electricity produced - the so-called marginal electricity mix - to the plant which is responsible for the additional demand.

What seems to be simple, may in practice be quite complex. In open electricity markets, increase of power generation occurs theoretically along merit-orders. The higher the current demand, the higher in general the marginal cost of the power plants getting additionally into operation. Keeping in mind the volatility of non-claimed renewable power, the merit-order curve is shifted over time. The more renewable power is produced, the more the merit-order curve is shifted towards higher demands, i.e., the same conventional power plant would only start into operation at higher demands compared to a point in time with low contribution from renewables, and vice versa. Current level of renewable power production and demand thus would have to be considered in any case.

In addition, it is important to recognise that real electricity markets are not ideal. For various reasons, some power plants are not contracted ideally along a merit-order. Some of them are even operated vastly

independent of any merit-order. For example, in industry, many companies operate their power plants like this. In the steel industry, power plants are mostly operated according to the incidental amount of residual gases from steel making. In the chemical industry, many sites run their own power plants in a CHP (Combined Heat and Power production) mode which is determined by heat (especially steam) demand. The rate of power production is thus driven rather by the demand of heat than by electricity markets. Besides, some conventional power plants may be operated independent of any price signal along a merit-order at least at a specific minimum load just to be able to provide control power, a service for grid stability.

In total, it may be laborious already retrospectively to derive time-resolved data for the marginal electricity mix. Even more challenging is to derive prognostic data, for example, to support decisions about times of preferred operation.

A separate issue results in case of large-scale roll-out of technologies implying additional power demand. In this case, not a single power plant but a multitude of power plants, possibly of various kinds and specific emissions, could be needed to cover the total additional demand in some times. It thus would be meaningful to estimate the total amount of additional electricity and allocate the average of emissions to all additional electricity consumed.

Such desirable models and tools are not yet available for practitioners, neither retrospectively nor for prognoses. It is thus strongly recommended to develop corresponding solutions (beyond the scope of this work). In line with the elaboration for renewable electricity, those solutions should also include spatial effects and potential limitations in transmission line capacities and interconnectors between countries. Even simplified models using approximations of the real world could already be better than to use static data, averaged across all non-claimed power production and/or assuming that Europe is electrically a copper plate.

In the meantime, as a kind of minimum standard, annually averaged national residual mix data **shall** be used in LCA for all cases of demand for unspecified electricity. The latest national residual mix data can be found here: <https://www.aib-net.org/facts/european-residual-mix>.

As long as (either time-resolved or annually averaged) marginal electricity mix data is not yet available, it is recommended to apply a scenario analysis based on the case that residual grid mix data is cleared up for nuclear and (non-claimed) renewable electricity.

Use of annually averaged data across all kinds of power generation including claimed electricity and especially renewable electricity, **shall not** be allowed.

9.3.5 Concluding remarks

As the elaboration in section 11.3 shows, electricity is a complex matter, necessitating review of LCA modelling procedures. Although very challenging, there is no alternative to develop improved solutions and consequently apply them. Otherwise, big differences in LCAs may persist because practitioners apply separate models and assumptions. CCU may for example make perfect sense in cases of very high availability of renewable electricity but only little sense if any at all under severe constraints of availability of renewable electricity.

Besides potential shortcomings of adequate electricity-related models for LCA, there are further unsatisfactory aspects which are rather out of scope of a single practitioner in the area of LCA for CCU. A few examples are presented for illustration:

- The guidelines presented here do not yet necessarily apply to all areas of LCA. For example, in other applications, power demand may be modelled and assessed conventionally using grid mix data. Whenever CCU technologies are compared to non-CCU processes or derived products, a lack

of comparability could result and special care should be taken. A prominent example is comparison of sustainable mobility via CCU-based fuels and via Battery Electric Vehicles (BEV). Often, BEV are assessed using annually averaged grid mix data. Neither time-dependent nor residual grid mix data are used. This could lead to wrong conclusions in direct comparison with mobility based on CCU-fuels being assessed under the guidelines presented here.

- Currently, EU member states report electricity-related emissions according to production within the national borders, not dependent on consumption. All electricity imported thus counts as burden-free. This is clearly inconsistent with general modelling of LCA where emissions would be attributed independent of borders between countries.
- The elementary recommendation to model and balance cradle-to-grave is often not considered in important policies. For example, indirect emissions were not adequately represented in FQD default values for hydrogen and SNG produced by electrolysis using renewable electricity. Likewise, instead of balancing mobility cradle-to-grave (well-to-wheel), separate regulations exist for fuels (well-to-tank) and for vehicles (tank-to-wheel). Regardless of whether there are historical or other reasons for such directives, it is impossible to overcome corresponding inconsistencies by whatsoever best LCA methodology and practice.

9.4 Selected other sources than renewable electricity for low-carbon intensity H₂

In the case of the use of H₂ in a CCU process, besides production of hydrogen from electrolysis by use of renewable electricity, alternative options with reduced environmental impact exist. For some of those energy sources, it is meaningful to also provide guidance with respect to LCA for CCU.

9.4.1 H₂ from Natural Gas via SMR+CCS or via Pyrolysis

Not least because of lack of availability of renewable electricity today and in the near future, hydrogen production via alternative options from natural gas such as Steam Methane Reforming (SMR) combined with Carbon Capture and Sequestration (CCS) or pyrolysis of natural gas into hydrogen and solid carbon has gained increasing interest in the recent past. As long as additional electricity demand is incurred, e.g., for compression of CO₂ for sequestration or in case of plasma-based pyrolysis, all recommendations in section 11.3 for electricity **shall** apply.

In addition to this, it is necessary to refine modelling of natural gas within LCAs. Depending on origin and transport mode of natural gas (consider for example Russian pipeline gas vs. LNG from US Shale Gas) its related environmental impact may vary significantly. This is of special relevance in the context of low-impact hydrogen making. Use of averaged data for LCA modelling of natural gas could be misleading. Instead, LCA **should** apply origin-specific data and explain how use of the related natural gas will be ensured in practice. Deviation from this guideline **shall** be justified and documented.

9.4.2 H₂ as co-product from industrial processes

Several industrial processes exist with hydrogen as a co-product. Examples are chlorine-alkali electrolysis, hydrocrackers in petrochemical plants and coking plants in steel mills. In an attempt to overcome both economic entrance barriers for CCU technologies as well as constraints of availability of cheap renewable electricity, it is sometimes of interest to use such hydrogen as a bridge to a future world with higher availability of cheap renewable power. On the one hand, the approach is comprehensible, on the other hand, thorough assessment of such solutions is necessary in order to avoid environmentally counter-

productive use.

It is of general interest, how to allocate emissions of the generating plant to the H₂ being used by the CCU plant. H₂ is typically not the main product of the generating plant. The situation is thus somewhat similar to the cases of CO₂ as feedstock (section 11.2). Again, consequential modelling provides the general framework for concrete guidelines. Typically, co-produced hydrogen from an existing plant is used chemically, e.g., for hydrogenation, or for heat and/or power production. Upon use of the hydrogen instead for CCU, the reduction in product of the reference system (i.e., in the examples above H₂ by itself, heat and/or power) **shall** be compensated arithmetically by corresponding system expansion, i.e., inclusion of a new source for the same amount of those products) and the corresponding emissions. Those additional emissions occur upon operation of the CCU plant and hence **should** be allocated completely to the CCU plant. In case of deviation from this general rule, this **shall** be justified and documented.

The case of a H₂ co-producing plant which is to be built together with a CCU plant, needs additional consideration. Since, as already stated, H₂ is not the main product, the H₂ co-producing plant will most often be installed and operated to produce the “other” product. LCA **should** thus assume as a reference system the same H₂-co-producing plant (to be newly-built) but with conventional use of H₂, i.e., not for CCU. For both, the H₂ co-producing plant as well as the fictitious plant for conventional use of H₂, Best Available Technology **should** be assumed including scenarios or sensitivity analysis for future development in BAT. Again, any deviation **shall** be justified and documented.

9.5 Use of otherwise lost heat

Sometimes, heat for a CCU process such as for recovery of a sorbent in the CO₂ capture process is provided by the primary CO₂ emitting plant. If the heat was used prior to installation and operation of the CCU plant for other technical purposes, e.g., power production or district heating, it may be referred to section 11.2 regarding guidelines for LCA. In specific cases, however, there hasn't been a technical use for the respective heat of the primary CO₂ emitting plant. The case is illustrated in Figure 20. For example, some heat from steel mills or other industrial furnaces is not exploited according to BAT (Best Available Technology). The question arises as to how to deal with such heat once it is being technically used in the CCU plant. Again, it is meaningful to differentiate between existing plants and those to be new-built together with a CCU plant.

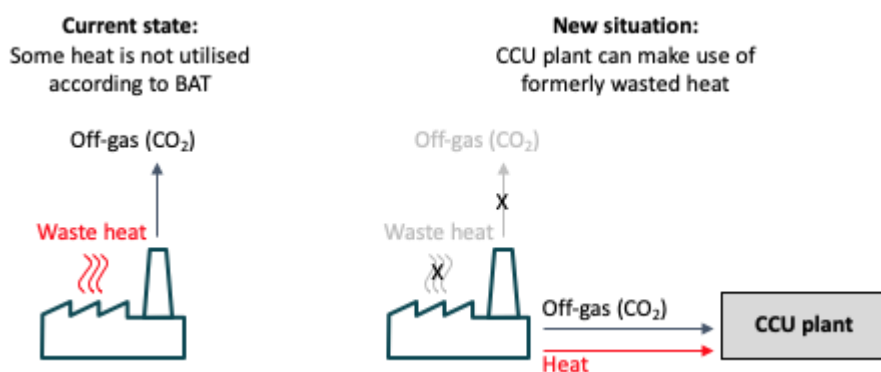


Figure 20: Schematic setting of CCU plant exploiting heat from a separate source where the heat has not been utilised so far

In general, it is of relevance whether it is in line with Best Available Technology (BAT) that the respective heat is not technically utilised so far. In this case LCA **should** assume that the heat is free of emission burdens for the CCU plant. Otherwise, the LCA **shall** use a reference system according to BAT where the reduction in provision of heat (upon operation of the CCU system) is to be compensated for accordingly by the addition of a separate source of heat.

A complicating factor is that BAT may be site-specific. For example, in the case of a district heating system next to the heat emitting plant, BAT may include exploitation of the heat for the heating system. In case there is no such sink for low temperature heat in the vicinity, BAT may exclude the use of the heat. It may thus be necessary to take a differentiated look at this matter within an LCA. In case heat is treated burden-free, LCA **shall** thus include in addition a differentiated analysis of BAT with respect to site-specific boundary conditions. This analysis **should** further include not only the site-specific situation at the starting point in time of the CCU plant but also future perspectives.

In case the heat emitting and the CCU plant will be new-built together, the requirements regarding differentiated analysis of BAT are even higher. In the framework of general efficiency improvements in the future, it has especially to be questioned whether loss of heat will still represent BAT in the future. Respective considerations and conclusions **shall** be documented in the LCA.

10 Impact Categories

10.1 General

Life cycle impact assessment is covered by EN ISO 14040:2006 (chapter 5.4) and EN ISO 14044:2006 (chapter 4.4). Provisions of these standards **shall** apply to life cycle impact assessment of CCU products.

10.2 Impact Categories to Consider

It is extremely important to state that climate change is not the only impact category that should be considered within an LCA. Whilst the purpose of CCU is to use CO₂, other impacts must not be forgotten. For a start, the significant amount of energy used will lead to impacts under various impact categories. Therefore, to ensure that any LCA for a CCU system is a real LCA and follows the guidelines of the ISO 14040 and ISO 14044 standards, all relevant impact categories **should** be considered. In terms of relevance, before undertaking an analysis, it is very difficult to know what is relevant. Hence, we recommend that given the relatively low level of experience in CCU (as discussed in chapter 10), the maximum impact categories are considered, within the limits of the knowledge of the system.

The selection of impact categories has to be in line with the Goal and Scope definition. CCU often aims at reducing CO₂ emissions and uses CO₂ as an alternative source of carbon. So, the assessment of impacts on global warming and on fossil resource depletion **shall** always be included in the scope of LCA for CCU. However, the development of CCU technologies may affect a variety of environmental impacts and the main goal of LCA is to identify transfer impact. So, to identify transfer impact, impact categories **shall not** be omitted from LCA studies if they are relevant i.e. accounted elementary flows which contribute in these categories and accessible i.e. impact assessment methods exist and these methods are reliable.

Below are impact categories adapted from the Joint Research Council's methodology:

- Quality level I: Global warming – Ozone depletion – Particulate matter/respiratory inorganics (I/II)
- Quality level II: Ionizing radiation, human health – Ionizing radiation, ecosystems – Photochemical ozone formation – Acidification – Eutrophication, terrestrial and aquatic – Resource depletion, mineral and fossil – Human toxicity, cancer and non-cancer effects – Ecotoxicity, freshwater – Resource depletion, water

The quality levels are as follows:

I: recommended and satisfactory,

II: recommended but to use with caution

The best practice is to look at the following full list of impact categories:

- Acidification
- Climate change (biogenic, fossil, Land)
- Ecotoxicity, freshwater (inorganics, metals, organics)
- EF-particulate Matter
- Eutrophication (marine, freshwater, terrestrial)
- Human toxicity, cancer (inorganics, metals, organics)
- Human toxicity, non-cancer (inorganics, metals, organics))
- Ionising radiation, human health
- Land use

- Ozone depletion
- Photochemical ozone formation - human health
- Resource use, fossils
- Resource use, minerals and metals
- Water use

The selection of a smaller list **shall** be justified. One impact category **shall** not be chosen to be consistent with an LCA , multicriteria assessment.

The use of CML impact categories is recommended, on the basis that this will harmonise with the International Environmental Product Declaration (EPD) System.

For low TRL technologies, where it is particularly difficult to gather information, it is important to at least include emissions to air, marine water, freshwater and land.

Whilst a study may use endpoints if the practitioner wishes, they must always use midpoints in order to offer some level of comparability with other studies.

In general, indicators at endpoint level are sometimes considered to lead to more understandable results; which is connected with the environmental relevance of the indicators. Levels of uncertainty increase with the use of endpoints, and it is extremely important to clearly state these levels of uncertainty. The choice of endpoint level should be linked to the goal and scope of the study.

For mid-points level, guidelines provided by PEF (Product Environmental Footprint) should be considered

10.3 Future Impact Analysis

Data on all major emissions **should** be provided in life cycle inventory, not just an impact category, to allow recalculation with new data (such as when AR6 is released in 2021).

10.4 Water Use Issues

Water consumption should take into account a local element, as a large water use in Scotland, for example, is not an issue. Whereas in Namibia this could be considered a major issue.

We recommend that LCA practitioners use the now widely used method of the AWARE method (Available Water REmaining). This methodology and the data sources is contained within <http://www.wulca-waterlca.org>, developed within ²¹ and ²²stress all water types

²¹ Müller Schmied, H., Eisner, S., Franz, D., Wattenbach, M., Portmann, F. T., Flörke, M., and Döll, P. (2014): Sensitivity of simulated global-scale freshwater fluxes and storages to input data, hydrological model structure, human water use and calibration, Hydrol. Earth Syst. Sci., 18, 3511-3538, <http://dx.doi.org/10.5194/hess-18-3511-2014>

²² Martina Flörke, Ellen Kynast, Ilona Bärlund, Stephanie Eisner, Florian Wimmer, Joseph Alcamo (2013): Domestic and industrial water uses of the past 60 years as a mirror of socio-economic development: A global simulation study, Global Environmental Change, Volume 23, Issue 1, February 2013, Pages 144-156, ISSN 0959-3780, <http://dx.doi.org/10.1016/j.gloenvcha.2012.10.018>

10.5 Climate Change Specific Issues

10.5.1 GWP20

Generally, a 100-year time window is used for the Global Warming Potential of emissions, referred to as GWP 100. This is used, as when the initial Intergovernmental Panel on Climate Change (IPCC) report was released, globally the concept of 100-year time periods for CFCs was understood after the success of the Montreal Agreement on CFCs. Therefore, politically, it was chosen as a good concept to allow policymakers to understand the concepts on climate change being published. It is important to state there is no scientific reason for the use of GWP100, it was purely to help policy makers within the 1990s.

It is important that both 20 year and 100-year climate change impacts are considered. This is on that basis that the climatic system is possibly on the verge of the activation of various feedback cycles which could lead to runaway climate change. On the other hand, it is unwise to simply reduce the timescale to 20 years for the impact category, as this could then incentivise other emissions and lead to poor decision-making processes. Therefore, we propose the use of both 20 year and 100-year GWP impact categories. The figures for GWP20 are given within the same IPCC reports that GWP100 is sourced from.

10.5.2 Delayed Emissions

Delayed emissions are a serious consideration for CCU, as due to the sheer range of products, then some of these will contain the carbon atoms for a long period of time, whereas others will release the carbon back into the atmosphere quickly (Figure 21). An example of where the carbon returns quickly to the atmosphere would be a fuel produced by CCU, however, other materials, such as plastics, may take a longer period of time to emit back into the atmosphere. This could be 20 or 30 years perhaps. With a greater understanding of bacteria breaking down plastic in the oceans, turning the masses of waste plastic within the oceans into a new possible source of greenhouse gas emissions, then this could be storage for as little as a few years. Ultimately, it will depend on the use of the plastic and the type of disposal. Furthermore, some CO₂ will be locked up as minerals, at which point it is long term storage which could be considered simply CCS, although this is a semantic issue.

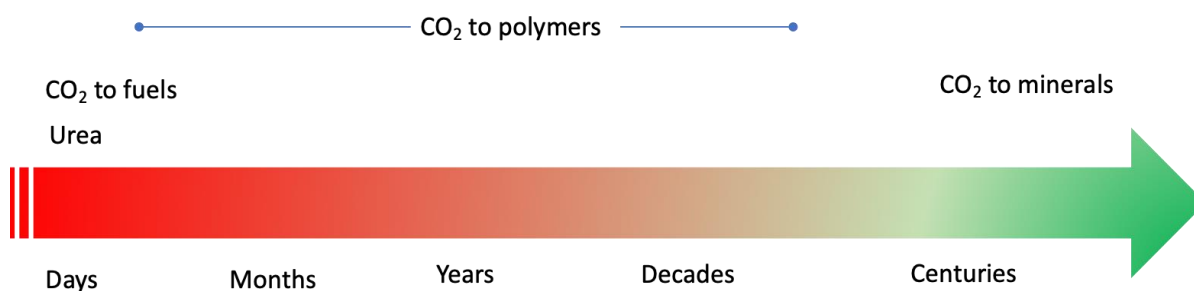


Figure 21: Horizon time of CO₂ emissions from CO₂ based products

There are numerous methods within academia and various standards on how to deal with delayed emissions. Detailed approaches include Levasseur et al 2010²³, in which the dynamic GWP is considered based on reworking the Radiative Forcing (RF) of the emissions of gases within a time window to create a combined figure for GWP through integrating under the RF from the pulse against time. However, a major concern with these methods is that they do not consider the future state of the global climatic system. An emission which is delayed by 50 years may be then emitted at a point where the climatic system is far less

²³ Dynamic LCA and Its Application to Global Warming Impact Assessments, Annie Levasseur, Pascal Lesage, Manuele Margni, Louise Deschênes, Réjean Samson, Environ. Sci. Technol.2010, 44, 8, 3169-3174, <https://doi.org/10.1021/es9030003>

stable than today. Conversely, it could be considered that delaying an emission delays the point at which the climatic system becomes extremely destabilised and positive feedback cycles take the earth's climatic system into a new state which could cause significant issues for human society. Depending on the time window considered, an emission could still cause significant issues in terms of climate change whilst not actually showing up within the LCA. We also have concerns that any method of giving credits for delayed emissions will in some way accidentally incentivise medium term (~100 year) storage, releasing CO₂ emissions in a future when it would be the worst time for further pulses in warming.

Therefore, we have chosen to avoid the more complex methods, as the uncertainties and risks of incentivising emissions are too great. Hence, we have decided on a single proposal, where we take a 500-year horizon as a point where we consider either society will have solved the issue of climate change and hence pulses of delayed emissions will not be an issue, or that climate change will have reached such an uncontrollable and dangerous state that the delayed emissions from society in the 21st century will pale its significance to the problems society will be facing by the 26th century.

10.5.3 Ensuring harmonisation within GWP impacts

In addition to considering the methodology that should be used for stored carbon, and the issues in terms of timescales, furthermore, the correct data for GWP should be used. With every major IPCC report, the figures for the Global Warming Potential of different gases are updated, this is due to a greater understanding of the chemical and biogenic processes experienced by greenhouse gases. However, there is a significant lack of consistency in terms of the versions which are used. The most commonly used version of the IPCC figures comes from the Fourth Assessment Report (2007)²⁴. Less commonly, the values from the Third Assessment Report (TAR) 2001²⁵ are used, whilst very rarely, the up to date figures from the 2013 Fifth Assessment (AR5)²⁶ are used. In 2021, the Sixth Assessment (AR6) will be released, presumably with different values again. This can have an impact on results, for example, as shown by the work within the All-Gas project, this can in certain cases lead to a 10% difference in GWP values (in the case of AR4 versus AR5).

To show the differences, let us consider the most well used gases with the RED and most basic carbon footprinting exercises, carbon dioxide, methane and nitrous oxide. We present below the impacts of these gases in terms of 20-year and 100-year climate change impacts.

Table 4: Figures from TAR, AR4 and AR5. Note, the AR5 figures are for fossil methane, biogenic methane provides figures of 28

²⁴ [2] Solomon S, Qin D, Manning M, Chen Z, Marquis M, Averyt KB, et al. IPCC, 2007: Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge, United Kingdom and New York, NY, USA: Cambridge University Press; 2007.

²⁵ O. Boucher, J. Haigh, D. Hauglustaine, J. Haywood, G. Myhre, T. Nakajima, G.Y. Shi, S. Solomon, 2001: Radiative Forcing of Climate Change. In: Climate Change 2001: The Scientific Basis. Contribution of Working Group I to the Third Assessment Report of the Intergovernmental Panel on Climate Change [Houghton, J.T., Y. Ding, D.J. Griggs, M. Noguer, P.J. van der Linden, X. Dai, K. Maskell, and C.A. Johnson (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 881pp.

²⁶ Stocker TF, Qin D, Plattner G-K, Tignor M, Allen SK, Boschung J, et al. IPCC, 2013: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change. Cambridge, UK and New York, USA: Cambridge University Press; 2013.

kgCO_{2eq}(GWP20) and 84 kgCO_{2eq}(GWP100)

Report	20 Year Global Warming Potential [kgCO _{2eq}]		100 Year Global Warming Potential [kgCO _{2eq}]	
	CH ₄	N ₂ O	CH ₄	N ₂ O
TAR (2001)	62	275	23	296
AR4 (2007)	72	289	20	298
AR5 (2013)	85	264	30	265
TAR/AR5	0.73	1.04	0.77	1.12
AR4/AR5	0.85	1.09	0.67	1.12

There is a clear difference, however, there are discrepancies between the two. There is still uncertainty about the methodologies used within the carbon-climate feedback, which is the reason given by the team behind RED II for using outdated data. An important point is that in terms of, for example, methane leakage from natural gas facilities the use of older data gives these facilities an artificially low impact.

It is interesting to note the RED has a history of using outdated data, in 2021, the the AR6 report from the IPCC will come out, showing as the RED keeps figures which are two reports back in the IPCC cycle.

However, where AR5 is used within the LCA community, there are issues with the consistency of AR5. ReCiPe 2016, EcoInvent IPCC 2013 and GaBi's AR5 database all show inconsistencies in the way their AR5 data was implemented. These include inconsistencies on the accuracy of figures, the list of gases considered, and issues arising from carbon-climate feedbacks, as well as an understanding of the data within the AR5 supplementary material, which is not part of the main report.

AR6 will also have similar issues, the EU should ensure that there is a single database between different software packages, and between the IPCC. There is already an embryonic working group between software developers and the industry, which could be given support and recognition by the EU Commission, and could feed accurate up to date figures through to multiple LCA based European Commission initiatives, including this work on CCU, as well as ensuring that RED begins to use up to date climate change data.

10.6 Recommendations

Based on the above, we make the following recommendations.

In terms of the impact categories, these **should** use the latest version of the full set of CML mid point impact categories. Whilst we do not recommend against using more impact categories, if the practitioner wishes to use fewer impact categories, then a justification should be given. It **shall** always be clear which impact categories are used, including the name of methodology, version, and date released.

In terms of climate change, practitioners shall use the latest values from the IPCC for GWP. In the year 2020, these figures from the IPCC Fifth Assessment Report (AR5), but after April 2021, these shall come from the IPCC Sixth Assessment Report (AR6). When using Global Warming Potentials, the standard 100 year time horizon **shall** be used, but also the 20 year time horizon figures **shall** be used. For delayed emissions, if the emissions are emitted within a 500 year time window, then they **shall** be assumed to be emitted at year zero. However, if they are emitted outside of this 500 year window (to a reasonable level of certainty), then they **should** be ignored.

11 Uncertainty analysis

One of the most important uses of LCA is to support decision-making regarding future course of action. Future decisions may concern for instance which technology to further develop or what part of the life cycle of a process or service is especially problematic and requires further attention. Future decisions will be better decisions if they include not only the (numerical) outcomes of the LCA but also the uncertainty in these outcomes, that is how likely is that the outcomes are right or wrong. Despite or maybe because of its importance, uncertainty management remains a key challenge in life cycle assessments, especially for technologies at (very) early stage of development (i.e. low TRLs).

Uncertainty is difficult to define and there is not a unique definition commonly accepted. Typical definitions found in the literature include:

- “Incomplete information about a particular subject”²⁷
- “Lack of confidence in knowledge related to a specific question”²⁸
- “Any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system”²⁹

Uncertainty is in fact most frequently defined through classification and several studies have provided a number of taxonomies to classify different types of uncertainty^{30,31}. Although there is a lack of consensus about the definition, classification and operationalization of uncertainty, there are common threads that can be identified, namely:

- Uncertainty is unavoidable
- Uncertainty is not simply the absence of knowledge
- Uncertainty is either chronically understated (to e.g., promote consensus) or overemphasized (e.g., to prevent action)
- Uncertainty has quantifiable and non-quantifiable components
- Uncertainty has reducible (e.g. stemming from erroneous knowledge or data) and irreducible (stemming from inherent variability) components
- Reducible and irreducible components of uncertainty have ‘fact’ and ‘linguistic’ components. In other words, uncertainties associated with (i) the robustness of the data/facts on which knowledge is constructed and (ii) with the way in which knowledge is formulated (i.e., the terms used to express (the lack of) knowledge, results, assumptions, etc.)

²⁷ Ascough J.C., Maier H.R., Ravalico J.K., Strudley M.W., 2008. Future research challenges for incorporation of uncertainty in environmental and ecological decision making. *Ecological modelling* 219, 383-389.

²⁸ Siget K., Klauer B., Pahl-Wostl C., Conceptualizing uncertainty in environmental decision-making: the example of the EU water framework directive. *Ecological economics* 69, 502-510

²⁹ Walker W., Harremoes P., Rotmas J., van der Sluijs J., Asselt M., Janssen P., Krayer von Krauss M., 2003. Defining uncertainty. A conceptual basis for uncertainty management in model-based decision support. *Integrated Assessment* 4 (1), 5-17

³⁰ Herrman I.T., Hauschild M., Sohn M.D., McKone T.E., 2014. Confronting uncertainty in life cycle assessment used for decision support. Developing and proposing a taxonomy for LCA studies. *Journal of Industrial Ecology* 18, 3, 366-379

³¹ Chapter 24 "The Nature of Uncertainty" in: Smithson, M., & Bammer, G. (2012). *Uncertainty and Risk: Multidisciplinary Perspectives*. Routledge.

- Uncertainty also has a ‘value-ladenness’ component, that is, it is sensitive to differences in subjective interpretations and the extent to which high stakes are involved
- Transparency of the results is improved by identified key sources and kind of uncertainties present, regardless of whether these can be reduced

In ISO 14044, uncertainty analysis is defined as a “systematic procedure to quantify the uncertainty introduced in the results of a life cycle inventory analysis due to the cumulative effects of model imprecision, input uncertainty and data variability”. Uncertainty analysis has therefore three main functions:

- (i) it provides insights into assumptions underlying the LCI;
- (ii) it gives an indication of model quality,
- (iii) it provides insights into the robustness of the outputs.

The adequate treatment of uncertainties implies that uncertainties salient for a decision-making process should be systematically identified, properly characterized and transparently communicated.

A challenge for any LCA is the many sources of uncertainty that can affect the robustness of the results. Generally, most uncertainty analyses in LCAs have focused on one type of uncertainty: uncertainty due to input data (also called parameter uncertainty). This includes, but is not limited to, data inaccuracy, data gaps, and unrepresentative data. The sources of uncertainties in an LCA are however broader and include among others³², model uncertainty, spatial variability, temporal variability, epistemological differences, and of course mistakes (easy to make, difficult to find). A combination of some or all of them are present in any LCA, and are therefore not exclusive of LCAs of CCU options. The main difference lies in the fact that whilst historically LCA has been predominantly retrospective in nature, that is, it has been applied to products and services that are already in the market, most CCU options are currently at an early stage of development and therefore they are concerned with the impacts of deploying a technology in the future. This increases the need and relevance of uncertainty analysis and management for understanding LCA results of CCU options.

Figure 22³³ schematically shows how degrees of freedom³⁴ (i.e. the possibility to alter and control (aspects of) a technology is higher at an early stage of development), costs (lower at early stage, higher at industrial stage) and data (lower at early stage, higher at industrial stage) develop over the different phases of technology development. As a result, the level of uncertainty in the LCA results will decrease as the technology develops (shown in dark green in the figure) due to increase in knowledge and data. Early LCA (also called prospective LCA or ex-ante LCA) does not result in lower uncertainties in LCA outputs (light green area in Figure 22), if anything the high level of uncertainty remains or increases. The explanation for this is quite simple: an ex-ante LCA is based on a scale-up of a lab concept to industrial scale because it is an industrial scale when the technology’s full environmental impact can be considered³⁵. Such scaling

³² Based on Björklund, A.E. Survey of approaches to improve reliability in LCA. *Int. J. Life Cycle Assess.* 2002, 7, 64–72.

³³ Villares M., Isildar A., van der Giesen C., Guinee J., 2017. Does ex ante application enhance the usefulness of LCA? A case study on an emerging technology for metal recovery from e-waste. *Int J Life Cycle Assessment* 22:1618-1633

³⁴ Generally defined as the number of independent variables that are free to vary to solve a given problem.

³⁵ Arvidson R., Timlan A.M., Sanden B.A., Janssen M., Nordelof A., Kushnir D., Molander S., (2017). Environmental Assessment of Emergent Technologies. Recommendations for prospective LCA. *J of Industrial Ecology* 22, 6, 1286-1294

requires using (very) limited data on the current performance of a technology at concept or experimental scale to extrapolate its further performance. Such extrapolation is generally based on a mix of real data, expert judgement and sometimes blunt guesses. The impacts estimated on data based at pre-commercial stage are, therefore, inherently uncertain and will substantially influence the impacts associated with a given process. These uncertainties cannot be avoided as they are inherent to the weaker knowledge base that is characteristic of process at an early stage of development. This is not to say that such LCAs are not useful. Prospective LCAs can provide insights into potential future performance, identify hotspots that could be tackled early on, and support selection of options and areas of further R&D. Outputs of prospective LCAs can therefore be used to actively shape technology development.

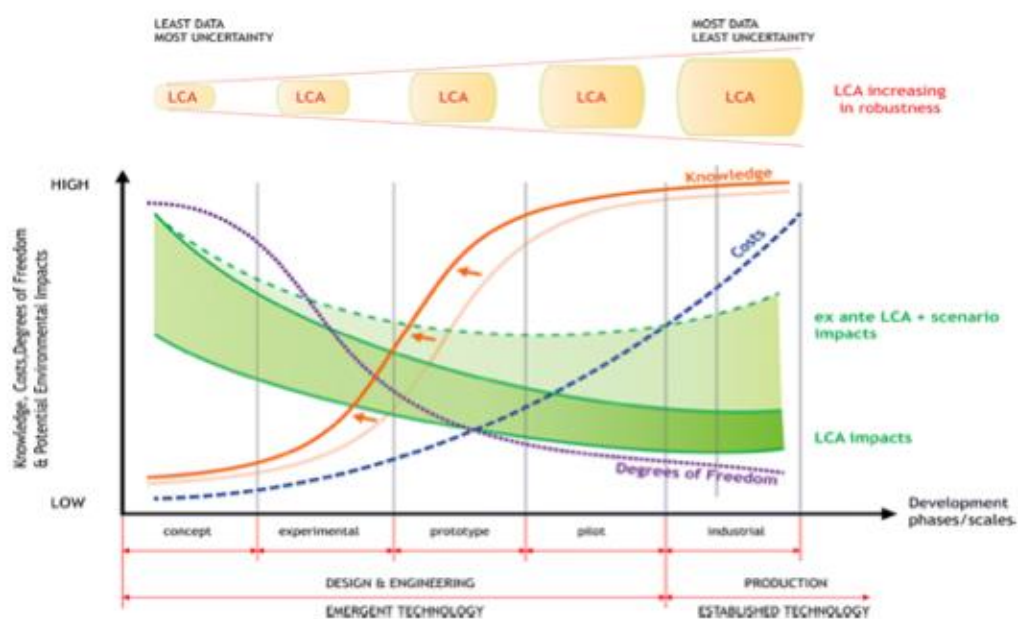


Figure 22: Uncertainty over a technology development path³³

11.1 Diagnostic vs Prognostic Uncertainty Analysis

What-if (diagnostic) assessments

What-if analysis is a way of simplifying the complexity of addressing the future performance of a technology in an LCA. Asking what-if questions provides a flexible and nuanced way to make uncertainty explicit. What-if questions are generally addressed through the use of scenarios. Scenario analysis copes with uncertainty by presenting a range of plausible futures, usually without assigning probabilities to the outcomes. Scenarios are not predictions. Rather, they are plausible stories about for instance how a technology (foreground processes) and or the rest of the world (background data and process in LCA) may develop in the future. In principle, scenarios can be used to assess the uncertainties regardless of the stage of development of a technology. However, if the uncertainty is relatively low (because e.g., the technology, location time, are already known) and the outcome is largely predetermined, the use of scenarios in uncertainty analysis and management will be less helpful. But, if the uncertainty is high (e.g., because the technology is currently at an early stage of development and therefore its future performance as well as the place and time where and when it will be deployed is unknown), the use of scenarios can provide useful insights. They provide a way to make potential changes in context variables explicit. An important outcome of a what-if analysis is therefore the identification of critical uncertainties: what aspects are most uncertain and will have the greatest impact on the outcomes?

An important condition to reach meaningful insights is for the scenarios to be internally consistent. For instance, if it is assumed that a CCU technology is going to be deployed in the future, let's say after 2030 and will use only renewable feedstocks (e.g., H₂) and energy sources (from e.g., wind, solar), the assumptions should also hold for the upstream and downstream processes of the LCA and should also guide the selection of the competitive (reference) technology. Furthermore, it is recommended that more than one scenario **shall** be explored. A single future scenario runs the risk of over (or under)-stating uncertainties that are identified as well as producing blind spots. A typical example is to limit a prospective LCA of a CCU technology to a single-scenario where the future technology (e.g., a CO₂-based fuel) is compared to today's technology (an oil-based fuel) and to assume that today's technology will be there tomorrow and it will do so in its current state (i.e., no further learning or improvement will be considered for the reference). This is not only internally inconsistent (in terms of scenario thinking as it creates a temporal mismatch between the novel technology and the reference technology) but also will not provide insights into the robustness of the outcomes (for instance, comparing the future CO₂-based fuel with a future competing technology that is not oil-based but electricity based, hydrogen based or bio-based, may result in significantly different outputs).

11.2 What-will (prognostic) assessments

The main difference between prognostic and diagnostic assessments is that while diagnostic assessments aim to explore the influence of inputs on outputs, prognostic assessments aim to predict the probability of a particular outcome as optimally as possible. Prediction requires detailed and strong knowledge about, for instance, the technology performance at the right scale, the location, the time, the upstream and downstream chain, the background system. Therefore, because the weak knowledge base inherent to technologies at an early stage of development (low TRL), the outcomes a prospective LCA (and their uncertainties) cannot, by definition, be prognostic. For technologies at high TRLs, in theory, it is possible to conduct a prognostic assessment, although the amount of specific data required and the level of general data that is available in LCA databases makes it very difficult to carry out and verify.

A main problem currently found in some LCA (of CCU) in literature is not that those studies are scoped as prognostic but that because of the way uncertainty is handled and communicated, the users of LCAs have the false impression they are. For instance, by providing numeral outcomes with a large number of decimals which a user may misinterpret as a sign of precision; by comparing outputs without including uncertainty ranges thereby omitting for instance that small differences between comparative options may fall within their uncertainty ranges and therefore strong conclusions cannot be derived from such comparison; by using terminology such as "large", "significant", "minor" without defining what is meant by it; by failing to report the presence of uncertainties (beyond data), etc. It is therefore important that if a study is (or cannot) be prognostic in nature, the LCA modeler **should** take particular care in avoiding the impression of prognosis in any of the LCA phases, but especially in the LCIA and interpretation phase.

11.3 Aim for transparency

Communicating the uncertainty of an LCA study is therefore imperative to ensure its transparency and credibility. This includes clearly communicating the different components in uncertainty management: their identification, characterization (quantitative and or qualitative) and evaluation. LCA studies **shall** therefore at least systematically identify and communicate uncertainties regardless of whether they can be quantitatively analysed. In this context, Gavankar et al.³⁶ defined five criteria to effectively

³⁶ Gavankar S, Anderson S, Keller AA (2014) Critical components of uncertainty communication in life cycle assessments of emerging technologies—nanotechnology as a case study. *J Ind Ecol* 19(3):468–479

communicate the uncertainty of LCA to decision-makers, which are helpful as point of departure: (i) report uncertainty, (ii) provide context, (iii) develop scenarios when quantitative methods cannot be used, (iv) use a common language for the subjective definition of probabilities, and (v) facilitate access to uncertainty information.

11.4 Tools and approaches

It is not the intention of this section to go into detail in existing tools that can be used for uncertainty analysis. There are many methods to deal with uncertainty, especially with the quantitative components of uncertainty. Some methods are intrinsic to the tools used, while others aim to provide guidance to the user on the implications of uncertainties in the selection of parameters and interpretations of results. Table 5 aims to provide a sample of the type of tools currently available with a focus on the strengths and weaknesses of each.

Table 5: Example of tools and approaches currently available for uncertainty management^{37,38,39,40}

<p>Sensitivity analysis: aims at understanding the influence that independent input parameters have in a given outcome of interest. Frequently, one-at-a-time approaches are used for sensitivity analysis.</p>	
<p>Strengths</p> <ul style="list-style-type: none"> ● Gives insight into the potential influences of changes in inputs. ● Helps ranking across parameters according to importance for the accuracy of the outcome. ● Software for sensitivity analysis is widely available. ● Easy to use. 	<p>Weaknesses</p> <ul style="list-style-type: none"> ● It can be time intensive which may drive modelers to only assess a limited set of parameters thereby overlooking possible sensitive parameters. ● It does not require to assess how likely it is that specific values of the parameters will actually occur. ● It does not encourage to identify and analyze potential dependencies between parameters and probabilities that certain values will occur together.
<p>Error propagation equations ("TIER 1"): aims to quantify how uncertainties in model inputs propagate in the model calculations to produce an uncertainty range in a given model outcome of interest.</p>	
<p>Strengths</p> <ul style="list-style-type: none"> ● Requires very little resources and skills (but the choice of the aggregation level for the 	<p>Weaknesses</p> <ul style="list-style-type: none"> ● It has a limited domain of applicability (e.g. near-linearity assumption).

³⁷ van der Sluijs, Jeronen P., et al. "RIVM/MNP guidance for uncertainty assessment and communication: tool catalogue for uncertainty assessment." *Utrecht University*

³⁸ Walker W., Harremoes P., Rotmas J., van der Sluijs J., Asselt M., Janssen P., Krayer von Krauss M., 2003. Defining uncertainty. A conceptual basis for uncertainty management in model-based decision support. *Integrated Assessment* 4 (1), 5-17

³⁹ Cox, David & Baybutt. (2006). Methods for Uncertainty Analysis: A Comparative Survey. *Risk Analysis*. 1. 251 - 258. 10.1111/j.1539-6924.1981.tb01425.x.

⁴⁰ Groen A., Heijungs R., Bokkers e., de Boer I., (2014). Methods for uncertainty propagation in life cycle assessment. *Environmental Modelling and Software*, 62: 316-325

<p>analysis is an important issue that does require skills).</p> <ul style="list-style-type: none"> ● Quick (but can be dirty). 	<ul style="list-style-type: none"> ● The basic error propagation equations cannot cope well with distributions with other shapes than normal (but the method can be extended to account for other distributions). ● Leads to a tendency to assume that all distributions are normal, even in cases where knowledge of the shape is absent. ● Cannot easily be applied in complex calculations.
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Monte Carlo Analysis ("TIER 2"): is a statistical numerical technique for stochastic model-calculations and analysis of error propagation in (model) calculations

<p><u>Strengths</u></p> <ul style="list-style-type: none"> ● Provides comprehensive insight into how specific uncertainty in inputs propagates through a model. ● Is capable to cope with any conceivable shape of PDF and can account for correlations. ● Can be used in 2-dimensional mode to separately assess variability and epistemological uncertainty. 	<p><u>Weaknesses</u></p> <ul style="list-style-type: none"> ● Is limited to those uncertainties that can be quantified and expressed as probabilities. ● Does not require reasonable basis on which to ascribe a parameterized probability distribution to parameters. They remain subjective probability distributions. ● May take large run-time for computationally intensive models. ● The interpretation of a probability distribution of the results can be perceived as too complex by decision makers. ● Some software can only use normal distribution
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Pedigree Analysis: evaluates the strength of a number by looking at the background history of how the number was produced and the underpinning and scientific status of the number.

<p><u>Strengths</u></p> <ul style="list-style-type: none"> ● It identifies the different sorts of uncertainty in quantitative information and enables them to be displayed in a standardized and self-explanatory way. ● It is flexible in its use and can be used on different levels of comprehensiveness: from a 'back of the envelope' sketch to a sophisticated procedure involving structured informed in-depth group discussions on a parameter by parameter format, covering each pedigree criterion combined with a full-blown Monte Carlo assessment. ● The diagnostic diagram provides a convenient way in which to view each of the key parameters in terms of two crucial attributes: relative contribution to the sensitivity of the output, and their strength. 	<p><u>Weaknesses</u></p> <ul style="list-style-type: none"> ● The method is relatively new. There is as yet no system of quality assurance in its applications, nor settled guidelines for good practice. ● The scoring of pedigree criteria is to a certain degree subjective. Subjectivity can partly be remedied by the design of unambiguous pedigree matrices and by involving multiple experts in the scoring. The choice of experts to do the scoring is also a potential source of bias. ● The method is applicable only to simple calculations with (relatively) small numbers of parameters. But it may be questioned whether complicated calculations with many parameters are capable of effective uncertainty analysis by any means.
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<ul style="list-style-type: none"> ● It fosters an enhanced appreciation of the issue of quality in information. 	
<p>Expert Elicitation: is a structured process to elicit subjective judgments from experts. It is widely used in quantitative risk analysis to quantify uncertainties in cases where there is no or too few direct empirical data available to infer on uncertainty.</p>	
<p><u>Strengths</u></p> <ul style="list-style-type: none"> ● It has the potential to make use of all available knowledge including knowledge that cannot be easily formalized otherwise. ● It can easily include views of sceptics and reveals the level of expert disagreement on certain estimates. 	<p><u>Weaknesses</u></p> <ul style="list-style-type: none"> ● The results are sensitive to the selection of the experts whose estimates are gathered. ● The fraction of experts holding a given view is not proportional to the probability of that view being correct. ● There is however no good way to measure competence. In practice, the opinions are often weighted equally, although sometimes self-rating is used to obtain a weight-factor for the expert's competence.
<p>Scenario analysis: tries to describe logical and internally consistent sequences of events to explore how the future might, could or should evolve from the past and present.</p>	
<p><u>Strengths</u></p> <ul style="list-style-type: none"> ● Scenarios are often the only way to deal with the unknown future. ● Assumptions about future developments are made transparent and documented, ● Gives insight in key factors that determine future developments. ● Creates awareness on alternative development paths, risks, and opportunities and possibilities for policies or decision-making. 	<p><u>Weaknesses</u></p> <ul style="list-style-type: none"> ● The analysis is limited to those aspects of reality that can be quantified (quantitative scenarios). ● Difficult to test underlying assumptions (qualitative scenarios). ● Frequently scenarios do not go beyond trend extrapolation (quantitative scenarios). ● Frequently scenarios are surprise-free. ● Frequently models used contain only one view, which will make the outcomes narrow in scope, thus not doing justice to the wish to explore fundamentally different futures.
<p>Model Quality Checklist: aims to assist in the quality control process for environmental modelling.</p>	
<p><u>Strengths</u></p> <ul style="list-style-type: none"> ● It provides diagnostic help as to where problems with regard to quality and uncertainty may occur and why. ● It raises awareness of pitfalls in the modelling process. 	<p><u>Weaknesses</u></p> <ul style="list-style-type: none"> ● It identifies but does not analyse the importance of uncertainty.
<p>Pseudo-statistical approach: aims at enabling use of Monte Carlo simulations to simultaneously propagate uncertainty in unit process data and uncertainty due to the choice of allocation methods to LCA results.</p>	
<p><u>Strengths</u></p> <ul style="list-style-type: none"> ● Provide a systematic way to explicitly include 	<p><u>Weaknesses</u></p> <ul style="list-style-type: none"> ● Difficult to understand by non-experts.

and assess the impact of choices made (or driven by) stakeholders.

- Results are not straightforward to interpret.

11.5 Summary of Recommendations

Uncertainty analysis is a key in any life cycle assessment even more so when the topic of assessment is a novel technology that is not yet fully developed or introduced in the market, which is the case for most CCU technologies. In this chapter it is argued that examining the approach and quality of the uncertainty analysis of the LCA is actually a good indicator of the usefulness of the results. A key point of departure is transparency, therefore we recommend that any LCA of CCU **should** provide as a minimum a thorough report of uncertainties regardless of whether they can be (quantitatively) measured. The inventory should not only cover the data itself but also the models used (including the technical model), the background data, the reference scenario, etc. Furthermore it is important to be explicit about the goal of the LCA and its impact on uncertainty analysis, in other words, whether the LCA aims to answer what-if or what-will type of questions. Most LCAs of future technologies address the former (what-if) and therefore practitioners should be careful on creating the perception that what-will questions are addressed in their assessment. The selection of reference scenarios (in plural) is an important aspect of LCA of novel technologies and they should be temporally and spatially coherent with the technology of study (avoid using a technology of today as status-quo of comparison for a timeline far in the future). Basically, practitioners **shall** not handle (uncertainties in) the future as if it was the present. Finally, we recommend that when possible, a combination of quantitative and qualitative uncertainty methods should be used as they provide different insights into the types of uncertainties and their significance in the analysis.

12 Conclusions

This report provides Life Cycle Assessment (LCA) guidelines for Carbon Capture and Utilisation (CCU). As a point of departure, CCU is defined in this report as “those technologies that use CO₂ as feedstock and convert it into value-added products such as fuels, chemicals or materials”. The report does not aim to replace existing standards (e.g., EN ISO 14040 and EN ISO 14044), rather it departs from the standards and existing state-of-the-art knowledge in LCA to address points that are particularly relevant or critical for CCU.

The key strength of LCA is that the methodology can be applied to address the environmental aspects and potential environmental impacts throughout the life cycle of *any* good or service. Given this wealth of possibilities, it is however very important to precisely describe the research question to be answered. This may seem a trivial point but a review of LCA literature on CCU concepts already indicates that this point is sometimes overlooked or forgotten throughout the study (i.e. implications of a given goal setting at the start of the study do not match the methodological choices or conclusion drawn from the study). Since the goal definition is decisive for all the other phases of the LCA, a clear initial goal definition is crucial for a correct later interpretation of the results. It is thus recommended to pay particular attention to the goal definition since it affects the results and also the comparability of LCA studies. The present guidelines are intended to cover “decision support” situations according to the ILCD Handbook, therefore “accounting” cases are out of scope of the present guidelines.

The present guidelines require that “cradle-to-grave” **should** be the default system boundary to assess the environmental impact of a CCU technology. Only in this way, meaningful conclusions regarding carbon neutrality/negativity can be drawn in an unrestricted form. Other system boundaries are discouraged (“cradle-to-gate”) or even strongly discouraged (“gate-to-gate”), however, they **may** be chosen on the condition that a justification is provided and that the conclusions drawn from the study do not (explicitly or implicitly) expand or cover issues that can only be done with larger system boundaries.

The selection of the reference system plays an important role for understanding the potential environmental benefits (or pitfalls) of a CCU option. Because many CCU options are currently at low TRL level, the selection of a proper reference system remains challenging. In this guideline we recommend that more than one scenario **shall** be explored (such scenarios can include various reference systems, various backgrounds, etc). Selecting only a single future scenario (e.g., novel technology vs today's technology) runs the risk of over- (or under-)stating uncertainties that are identified as well as producing blind spots. When defining the scenarios care should be taken that they are both temporally and spatially consistent.

Regarding the impact categories, in this guideline we use CML Impact Categories but other categories may be used. It **shall** however be clear and explicitly reported which impact categories are used, including the name of methodology, version, and date released. Because one of the key values added by LCA is the potential to identify trade-offs among categories, here we recommend that all impact category types **should** be used, and if not, justification **shall** be given. Although the motivation of CCU often lies primarily in climate change and therefore many studies focus only on indicators related to greenhouse gases (e.g., Global Warming Potential), it is important for proper decision making to identify potential areas where trade-offs can occur as a consequence of CCU implementation. Furthermore, when looking at GWP, to understand short- and long-term impacts, both, GWP20 and GWP100, **should** be used. Finally, in this guideline we recommend that delayed emissions less than 500 years **shall** be treated as emitted at year zero, emissions delayed greater than 500 years (to a reasonable level of certainty) should be ignored.

In this guideline, we further recommend that system expansion **shall** be used. Sometimes however, allocation procedures are required, and as such allocation of CO₂ is one of the most relevant topics in LCA for CCU and also a potential pitfall. Very strict compliance to guidelines is essential along with very clear

communication of selected procedures at distinct places within the LCA and an assessment of the impact of allocation choices as part of the uncertainty analysis. Particular care should be taken to avoid that inadvertently emissions 'disappear' from the system, for instance by assuming that emissions are accounted for by a party that is outside of the system boundaries. In this guideline, we depart from a precautionary principle, which says that if the origin of the CO₂ to be used in the CCU options is not known or if the origin is known but there is no agreement on who has the burden of the emissions due to CO₂ capture and transport, the CCU system **shall** incorporate those into its system boundaries. Note that unless there is specific information about the source of the CO₂, it **shall not** be assumed that the flow is of non-fossil origin (i.e. CO₂ is considered of fossil origin unless information is provided which justifies to consider it biogenic or atmospheric).

Regarding impacts of (background) data, electricity tends to be much more relevant for most CCU applications than for others. Refinement compared to standard LCA is strongly recommended to improve quality of LCA for CCU, especially, it is important to consider impact of flexible operation on plant model and foreground data (e.g., if the system is assumed to use only intermittent renewables or is considered to provide an energy storage service to the grid); to further apply additionality and marginal electricity concepts, time-resolved data and to consider location of CCU plant and related potential grid restrictions.

Finally, uncertainty analysis remains an indispensable part of LCA and even more so for LCA of technologies that are not yet commercial. We recommend that whenever possible, a combination of quantitative and qualitative uncertainty methods should be used as they provide specific insights into the types of uncertainties and their significance in the analysis and that as a minimum, any LCA of CCU **should** provide a thorough report of uncertainties (in data, models, allocation choices, etc.) regardless of whether they can be (quantitatively) measured.

13 Outlook

Within this work, no general gaps in LCA methodology were identified in application to CCU. Instead, it showed that also for CCU, LCA is THE tool of choice for assessment of environmental impacts of technologies. Nevertheless, some topics are recommended for future work in the context of LCA for CCU to accelerate adoption of recommendations made within this report and to improve familiarity within the LCA community.

First, it seems generally very useful to develop and provide examples of LCA for selected CCU cases as best practice references. In this context, examples with high relevance, either because of the absolute amount of CO₂ emitted by the respective kind of source or because of the product market size (e.g., fuels, olefins, methanol, BTX aromatics, urea) could be of special interest.

Since often other, chemical energy containing gaseous components such as hydrogen or carbon monoxide come along with a CO₂ containing waste gas (as for example in steel mill waste gases), it is also worthwhile to validate applicability of the guidelines of this report on the example of such cases and - if meaningful or necessary - to expand the scope and/or add specific recommendations to the guidelines.

Also, it is already visible today that due to high dynamics in deployment of renewable energies and feedstock on the one hand and cut back of fossil energies and feedstock on the other hand as well as changes in state-of-the-art of industrial technologies and processes, continuous adjustment in timely manner of background data is essential for the quality and significance of LCA results. Higher frequencies of background data updates and validations may be necessary. This includes especially the mandatory use of most recent IPCC figures for any LCA for CCU.

As the background system will change so fast in the coming years, though at relatively high uncertainty, well defined and accepted scenarios for selected reference systems will be needed as a basis for practitioners to enable efficient execution of LCA as well as comparability of LCA studies. Those reference systems should include the power system in general (including share and location of renewables, kind of renewables, level of grid development, time-dependent resolution of power production and general demand) as well as state-of-the-art for selected key industrial processes, e.g. for steel, glass and cement making and production of selected base chemicals for selected points in time, e.g., by 2030, 2040 and 2050.

Furthermore, background data for carbon capture is currently not as well developed and available as it should be due to its relevance for LCA for CCU. Improvement regarding both quality and quantity of data in this area is strongly encouraged.

Due to the relatively high number of low TRL cases among CCU technologies, it is recommended to generally foster experience with treatment of uncertainty within LCA. Uncertainty in general is not a specific issue of CCU technologies. Yet, its relevance will in tendency be higher in the area of CCU. The common level of understanding and experience could be improved by dedicated research as well as a general stronger emphasis in future LCA.

The focus of this work has been on LCA aiming to support decision making. In the case of LCA aiming for accounting it may be desirable to apply allocation instead of system expansion which could cause deviations of results. There is no simple rule available today how to avoid such potential mismatches. It remains in the responsibility of the LCA practitioner to be aware of such differences and to consider them adequately in the interpretation of the results. Additionally, it might be useful to elaborate on selected examples how such mismatches could be avoided or at least a guideline how to deal with it.

There is a lack of relevant LCI data for CCU systems, and the individual relevant processes within such systems. We would welcome the development of LCI databases, which are platform independent, to support practitioners in the development analysis of CCU.

Beyond these recommendations, there are topics which fall out of the direct scope of LCA for CCU and/or require inclusion of additional expertise, nevertheless, it is anticipated that proper solutions would be of high value to ensure good fit between real operation of CCU plants and results from their respective models within an LCA study. For example, it would be meaningful to provide operators of CCU plants which are designed and intended to operate only in selected situations for marginal grid mix (e.g. at sufficiently low carbon footprint), with an online tool which enables them to predict within reasonable certainty the marginal mix over a reasonable period of time in the future (e.g., up to a day ahead). Also, it is to be clarified how - in the context of additionality - renewable power plants shall be treated which fall out of the regime of any public funding scheme but which will need some investment in refurbishment prior to continued use. Neither treatment as additional renewable power nor as already fully existing renewable power installation seems adequate. Further topics may come up within the context of future application of LCA for CCU. Finally, especially in the context of meso-/macro-level decision support by LCA and furthermore in cases which strongly rely on use of renewable electricity, it would be very meaningful to develop guidelines for how to assess the impacts of a large scale deployment of the respective CCU technology. Specifically, it would be very useful if information such as total renewable electricity demand, required transmission grid capacities, area demand for renewable power generation and transmission lines, impact of CCU plants and additional renewable power installations on availability of renewable power for other applications would be consistently developed and analysed in order to reflect future potential competition for renewable electricity, land use and grid capacity with other sectors.

Further issues which fall out of the scope of LCA for CCU specifically, but are important, are the issues highlighted in terms of the inconsistencies over the method used for climate change impacts, both the version issue (TAR, AR4, or AR5) and also the application of these methods. There needs to be greater work between LCA practitioners and the IPCC to resolve this issue.

14 Abbreviations

BAT	Best Available Technology
BEV	Battery Electric Vehicle
CCU	Carbon Capture and Utilisation
CCS	Carbon Capture and Storage
CHP	Combined Heat and Power (cogeneration)
DAC	Direct Air Capture
DRI	Direct Reduced Iron
EoL	End-of-Life
EOR	Enhanced Oil Recovery
EPD	Environmental Product Declaration
GHG	Greenhouse gas
GWP	Global Warming Potential
ILCD	International Reference Life Cycle Data System
IPPC	Intergovernmental Panel on Climate Change
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LHV	Lower Heating Value
LNG	Liquefied Natural Gas
OEF	Organisational Environmental Footprint
PCR	Product Category Rule
PEF	Product Environmental Footprint
PPA	Power Purchase Agreement
RED	Renewable Energy Directive
SMR	Steam Methane Reforming
SNG	Synthetic/Substitute Natural Gas
TRL	Technology Readiness Level

