THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

Looking at goals and scopes in LCA

Environmental assessment of carbon capture and utilisation for technology development

EVELINA NYQVIST

Division of Environmental Systems Analysis
Department of Technology Management and Economics
Chalmers University of Technology
Gothenburg, Sweden, 2024

Looking at goals and scopes in LCA
Environmental assessment of carbon capture and utilisation for technology development

EVELINA NYQVIST

This thesis has been prepared using LaTeX.

Division of Environmental Systems Analysis
Department of Technology Management and Economics
Chalmers University of Technology
SE-412 96 Gothenburg, Sweden
Phone: +46 (0)31 772 1000
www.chalmers.se

Printed by Chalmers digitaltryck/Chalmers Digital Print
Gothenburg, Sweden, 2024

Abstract

This licentiate thesis explores the goals and scopes of life cycle assessment (LCA) studies in the field of carbon dioxide capture and utilisation (CCU), within the context of technology development. In LCA, the goal of a study guides method choices, thus aligning the assessment and the interpretation of results to its purpose. This is especially important for emerging technologies like CCU, where early-stage LCA studies can influence development in stages characterised by uncertainty. Understanding the goals and scopes of LCA studies is essential, particularly if results are to effectively inform technology development. For this, the research builds on a methodological review of published LCA studies of CCU systems, focusing on their goal definitions and scope definitions. In addition, a case study was performed via an LCA study on a specific CCU system, the $PYROCO_2$ process. In this case study, there was an emphasis on goal definition and its relation to knowledge needs in technology development. The results of the methodological review indicate that LCA studies of CCU systems often have unclear goal definitions, making results difficult to interpret. The LCA case study sets clear goals to address knowledge gaps in technology development and points to a need for multiple LCA studies to better inform on the many aspects considered during technology development. These findings suggest that separating goal definition from scope definition is useful, but current practices and guidance on defining and linking them are weak. Improving goal definition and its connection to scope is necessary for better methodological choices and clearer communication of outcomes.

Keywords: Life cycle assessment, goal and scope definition, carbon dioxide capture and utilisation, emerging technologies, technology development.

List of Publications

This thesis is based on the following publications:

[A] **Evelina Nyqvist**, Henrikke Baumann, Gulnara Shavalieva, Matty Janssen, "Methodological review of life cycle assessments of carbon capture and utilisation - Does modelling relate to the climate urgency?". Under review in Cleaner Environmental Systems.

[B] **Evelina Nyqvist**, Matty Janssen, "A life cycle assessment study informing the development of acetone production from captured carbon dioxide". Draft.

Acknowledgments

Funding from $PYROCO_2$, in the European Union's Horizon 2020 research and innovation programme under grant agreement No 101037009, is gratefully acknowledged. Thanks to everyone in the project consortium for making my research possible. A special thanks to work package 5 for the interesting discussions and productive collaboration.

I want to thank my supervising team: Matty, Kikki and Gulnara, for their support and invaluable feedback throughout my research. I am also grateful to my colleagues at Environmental Systems Analysis (ESA) for creating an environment for discussing research. Special thanks to those I have shared an office with, for creating a supportive and enjoyable work environment. Additionally, I want to acknowledge my colleagues at the Department of Technology Management and Economics (TME) for making the PhD journey more fun, especially the PhD students and the TME PhD Council.

Acronyms

CCU:	Carbon dioxide capture and utilisation
CCUS:	Carbon capture, utilisation and storage
CCS:	Carbon dioxide capture and storage
CDR:	Carbon dioxide removal
CO_2:	Carbon dioxide
DAC:	Direct air capture
GHG:	Greenhouse gases
H_2:	Hydrogen
LCA:	Life cycle assessment
NET:	Negative emissions technology
R&D:	Research & development
RQ:	Research question
TRL:	Technology readiness level

Contents

List of Figures

List of Tables

Part I

Overview

CHAPTER 1

Introduction

In life cycle assessment (LCA), it is often said that method choices depend on the goal of the study. The goal definition is important because it outlines the purpose of the LCA study, which the LCA practitioner needs to understand in order to make relevant methodological choices (Baumann & Tillman, 2004; Lindfors et al., 1995). If the goal of an LCA study is not clear, the subsequent LCA modelling and analysis will not be aligned with the intended purpose of the study. Consequently, the LCA results are not necessarily useful in the intended application without a clear goal with the LCA study.

When assessing emerging technologies, the goals become even more important due to the many questions about the new technology that can be asked. Furthermore, there are different method choices the LCA practitioner can choose from to answer these questions. Consequently, different types of LCA studies can be performed during the (long and complex) technology development process. Since a distinct goal for an LCA requires its own method choices, it is crucial to better understand how to match them to the knowledge needs during the technology development process by studying the goal and scope.

LCA can also guide the technology development at the early stages and consequently influence what direction the development takes. One issue with the assessment of emerging technologies, however, is the lack of information and real data, which leads to limitations in what can be said with certainty in the assessment. However, assessment in the early stages of development have high uncertainty but can have higher influence on technology development than later when design choices are locked (Arvidsson et al., 2017). It is known that there are different goals and uses of LCA in technology development (e.g., Bergerson et al., 2020; Gavankar et al., 2014; Hetherington et al., 2013; Thomassen et al., 2019), but there are not enough details provided on how to perform these assessments for specific purposes. Hence, LCA studies of emerging technologies could be more useful for technology development if the studies are done with purposes fitting the knowledge needs of the technology development process.

One emerging technology for carbon abatement and replacement of fossil resources is carbon dioxide capture and utilisation (CCU). CCU is one of the carbon-reducing or carbon sink technologies said to be needed in industry to fulfil the Paris Agreement (IPCC, 2023; UNFCCC, 2016). CCU systems are technologies that convert captured CO_2, in captured industrial flue gases or directly from the atmosphere, into new products, such as chemicals, fuels and materials (IPCC, 2018). In contrast to carbon capture and storage (CCS) or carbon capture, utilisation and storage (CCUS), the carbon is only stored for the time the product is kept in use as opposed to permanent storage underground or in minerals (IPCC, 2018). From a life cycle perspective, the carbon abatement of CCU technologies depends on where the carbon originally comes from and how the CCU product is used and for how long. Hence, these aspects need to be considered when assessing CCU technologies from the environmental perspective.

Given the complexities of the CCU system, including the various elements of the industrial system and the time aspect of carbon retention time, appropriate environmental assessment is important for guiding CCU technology development towards climate mitigation effectively. LCA has become an important tool (e.g., Aresta & Tommasi, 1997; Langhorst et al., 2022; von der Assen et al., 2013) in the development of CCU technologies to evaluate their effectiveness in reducing carbon dioxide emissions. Since different perspectives and methodological choices lead to different assessments, each serving its purpose and use, it is essential to improve understanding on uses for LCA in technology development and the related goals and scopes in these assessments.

The goals of the assessments determine the method choices, and all choices should be stated in the scope definition. Thus, the goal and scope are the starting points and the basis for understanding the types of LCA studies applied in the field of CCU. Goals and scopes are important for any LCA study, and particularly in the emerging field of CCU. This is because CCU systems are complex, and there are different knowledge needs during technology development. These knowledge needs determine different goals with the LCA studies. Therefore, CCU is a suitable empirical field to investigate goals and scopes in detail.

1.1 Aim and research questions

The focus of this licentiate thesis is on the goals and scopes of LCA studies, utilising the CCU domain as the field for examination and exploration. It aims to provide better understanding of the goal and scope definition phase in LCA, and insights into CCU assessments for technology development. The following research questions will help to achieve the aim of the research:

1. What is the current methodological practice of defining the goal and scope, respectively, in LCA studies of CCU? What are the different types of LCA studies applied in the field of CCU?
2. What are the different goals in LCAs of CCU for addressing different knowledge needs during technology development?

1.2 My introduction to the research

My doctoral studies started as a project focused on performing prospective LCA on a CCU process, the PYROCO$_2$ process in an EU-funded project. The initial research questions were focused on the environmental performance of the process as well as what it means to have a "positive" impact (which the project claims to have, producing so-called "climate-positive" products). Before doing any LCA, I started reading about how to do LCA on CCU systems, which there were several guidelines for (e.g., Langhorst et al., 2022; Müller et al., 2020; von der Assen et al., 2013). I also searched for all LCAs performed on CCU systems and started a literature review. In the beginning, I was mapping their results, products studied and system boundaries. In combination with the CCU-specific gudielines available, I was hoping to inform myself on which LCA methods to use in LCA studies of CCU, but could not find any clear answers.

Very early in my PhD studies, I also attended The International Conference on Negative CO_2 emissions, where I soon understood that this community's view on CCU was that it is not at all a negative emissions technology like bioenergy with carbon capture, direct air capture, afforestation, mineralisation etc. I saw a conflict with the results of the LCAs in my review, where net-negative emissions were sometimes presented. Similarly, the issue of falsely accounting for negative emissions in LCA studies had been previously discussed, by e.g., Tanzer and Ramírez (2019). Consequently, I tried to understand the different perspectives and choices of modelling the same CCU system that result in perceptions of negative emissions.

In the process of trying to understand the reviewed studies, their methodologies and communication of results, their goal definition came into focus. Knowing that everything in an LCA study depends on the goal definition, that should help explain the differing methodologies and results of the reviewed studies. So, that became the focus of my literature review and following case study.

1.3 Thesis outline

This chapter has specified the issue of goals and scopes investigated in this licentiate thesis. The following chapter (Chapter 2), offers a background on LCA as a methodology and CCU as a technology. Readers not familiar with LCA will find a short introduction to the methodology in section 2.1. Of interest to all readers, this section also specifically presents goal definition and scope definition, as well as LCA of emerging technologies, which are in focus in the licentiate thesis. For those not familiar with carbon capture, section 2.2 differentiates between various concepts in the field and provides explanations on what a CCU system entails in the context of this licentiate thesis.

Chapter 3 presents the research design of my project and the methods used to address the research questions. Chapter 4 summarises the results presented in the included papers. These results are analysed in Chapter 5 in relation to the research questions of this licentiate thesis. Chapter 6 discusses these findings in relation to existing knowledge about goal and scope in LCA, and Chapter 7 provides the final conclusions.

CHAPTER 2

Background

In this chapter, the theoretical background of the life cycle assessment (LCA) methodology and the carbon capture and utilisation (CCU) concept are expanded.

2.1 Life cycle assessment

Life cycle assessment is a method developed to understand the environmental impacts of a product or service (Baumann & Tillman, 2004). The different steps of the method are defined by the standard as goal and scope definition, inventory analysis, life cycle impact assessment and interpretation (ISO, 2006), see the LCA procedure in Figure 2.1. In the goal and scope definition, what will be assessed, for whom and how it is done is defined. The inventory analysis is the part where all the processes are mapped in a flowchart (the life cycle model in Figure 2.1) and data are collected. The mapped resource and emission flows are then characterised and categorised into different environmental impacts, such as global warming, eutrophication, human toxicity etc. The results of the calculations are interpreted by the LCA practitioner and often presented in graphs showing environmental impacts. The method is iterative and it is not uncommon that the goal and scope is adjusted after collection of data or impact assessment.

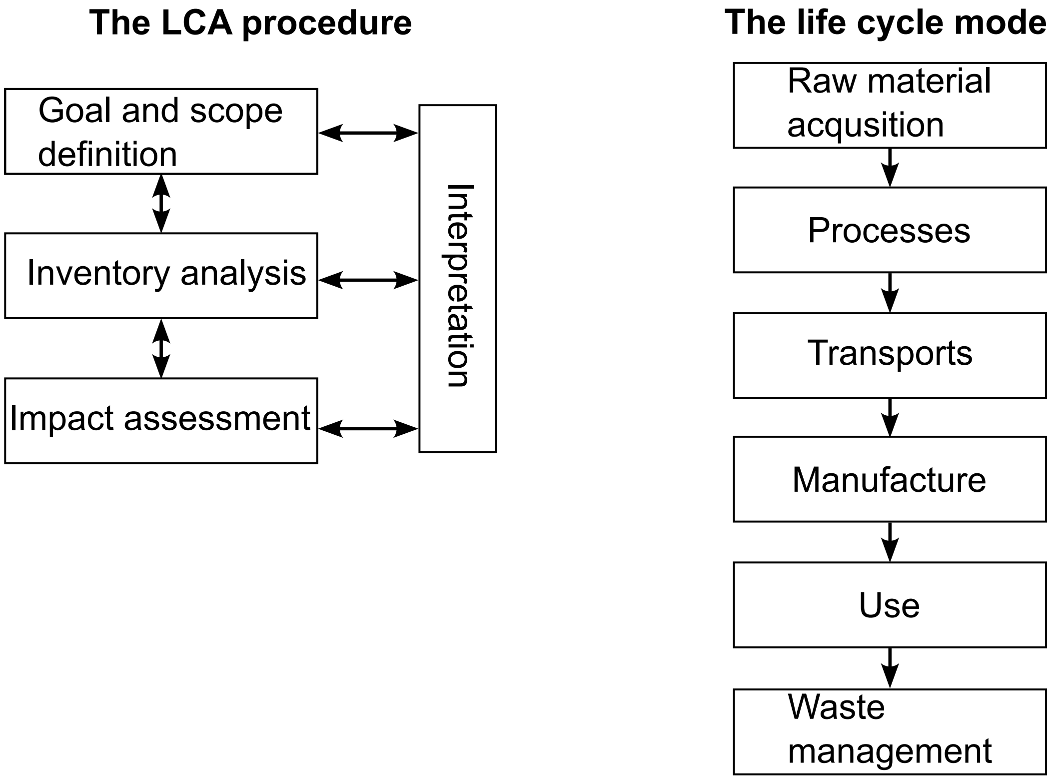

Figure 2.1: The LCA procedure and the life cycle model used in LCA. Adapted from (Baumann & Tillman, 2004).

The *goal and scope definition* is the first step of the LCA according to the ISO standard (ISO, 2006). Before the introduction of the standard, the first step was referred to as *goal definition* (Guinée et al., 1993) or *goal definition and scoping* (Lindfors et al., 1995). In both cases, it was directly followed by the inventory step, as in the current standard. The subtle difference between *goal and scope definition* and *goal definition and scoping* indicates that the current ISO standard treats the goal and the scope more as one unit (goal and scope) than previous terms suggest.

Although the standard and other guidelines provide direction for defining both the goal and the scope, they generally provide a list of items to consider without much detail on how to determine these considerations. A compiled list of these items is summarised in Table 2.1. The guidelines suggest that the scope should align with the goal of the study. However, they do not specify how the LCA practitioner should achieve this alignment, leaving much to the practitioner's judgement and expertise.

Table 2.1: Items of goal definition and scope definition. Based on Baumann and Tillman (2004), Curran (2017), and ISO (2006).

Goal definition	Scope definition
Purpose of the assessment	The studied product system(s)
The intended application	The studied system's function
The intended audience	The functional unit
Whether the results are for public comparisons	Choice of impact categories and impact assessment methodology
	Interpretation to be used
	Type of LCA
	Geographical system boundaries
	Time horizon
	System boundaries between technical and natural systems
	System boundaries relative capital goods
	Allocation procedures
	Data requirements
	Assumptions
	Limitations
	Type of critical review
	Type of reporting

Goal definition

According to several guidelines, the goal definition step is the first and most critical part of LCA (e.g., Baumann & Tillman, 2004; Klöpffer, 1997; Lindfors et al., 1995). The LCA practitioner needs to understand the specific and detailed purpose of the study, in order to make relevant methodological choices (Baumann & Tillman, 2004; Lindfors et al., 1995). The goal definition outlines the purpose of the study and its intended application (Baumann & Tillman, 2004; Bjørn et al., 2018; Lindfors et al., 1995).

To understand the purpose of the study, the LCA analyst needs to understand the needs of the commissioner. One way to define the goal of a study is to formulate the question(s) of the commissioner (Baumann & Tillman, 2004). The question(s) can be vague in the beginning of the study, but the study needs to have a specific purpose and the goal definition can be refined later (Baumann & Tillman, 2004). It is then the practitioner's role to decide the appropriate methodological choices, i.e., to determine the scope for the LCA model and analysis (Baumann & Tillman, 2004; Curran, 2017).

Bjørn et al. (2018), in their guidance on how to define the goal of an LCA study, distinguish between three types of decision-contexts (micro-level decision support, meso/macro level decision support and accounting). These different contexts inevitably lead to at least three different types of LCA. Types of purposes for LCA or uses for LCA have been categorised by Baumann (1995), depending on decision-making contexts (strategic decisions, construction and design, procurement and sales) and actors (authorities, companies, individuals, NGOs).

Scope definition

According to ISO (2006), the scope of an LCA study is defined in the same phase as the goal, during the goal and scope definition. The scope definition contains the specifications of the modelling, which should be consistent with the goal of the study (Baumann & Tillman, 2004). These specifications direct the following LCA work and include the choice of impact categories, time horizon, system boundaries, functional unit, data quality requirements, assumptions, limitations, type of review and reporting. Hence, the scope specifies how the whole LCA study is conducted.

LCA of emerging technologies

Technologies with radical novelty and fast growth are referred to as emerging technologies (Rotolo et al., 2015). LCA of emerging technologies is different from that of mature technologies (e.g., Hetherington et al., 2013; Moni et al., 2019). Due to uncertainties, data availability, smaller scale and comparability to conventional alternatives, LCA of emerging technologies becomes challenging and these complexities need to be considered (Hetherington et al., 2013).

LCA studies of emerging technologies are sometimes called prospective (e.g., Arvidsson et al., 2017; Thonemann et al., 2020) or ex-ante (e.g., Buyle et al., 2019; Cucurachi et al., 2018). In prospective LCA studies, the emerging technology is modelled at a future scale in a future time (Arvidsson et al., 2017). Other types of ex-ante LCA were listed by Cucurachi et al. (2018) as consequential, dynamic, anticipatory and mixed. Furthermore, Baumann and Tillman (2004) suggested different LCA approaches at different stages of product development, e.g., abridged LCA matrix for trend analysis or LCA-derived proxies for evaluation of components and details. Hence, there are several types of LCA studies that can be performed when assessing emerging technologies.

LCA of technologies at early development stages, i.e., at low technology readiness level (TRL) can be used to anticipate and detect possible environmental issues (Gavankar et al., 2014). The technology readiness levels (TRLs) is a scale from 1 to 9, ranging from basic principles observed to actual system proven (European Commission, 2017). While LCA at early development stages can be challenging due to uncertainty and lack of data, it can provide insights and guide decisions in the development (Hetherington et al., 2013).

It is suggested that LCA can have different uses at different TRLs (Bergerson et al., 2020; Gavankar et al., 2014; Thomassen et al., 2019) and can have different roles in technical research and development (R&D) (Sandin et al., 2014). The different LCA approaches listed by Baumann and Tillman (2004) can be applied at different stages of product development.

Consequently, the literature points to the existence of several types of LCA and various uses and roles of LCA in technology development. However, these types and uses are generally expressed and the guidance does not specify how to perform these assessments for the specific purposes.

2.2 Carbon capture and utilisation

Carbon capture, utilisation and storage (CCUS) is a group of technologies developed to reuse or store carbon dioxide to mitigate climate change impacts. Carbon capture and utilisation (CCU) is the process of capturing carbon dioxide (CO_2) and using it in the production of a product (IPCC, 2018). If the product stores the carbon for a "climate-relevant time", the process can be called carbon capture, utilisation and storage (IPCC, 2018). There are also carbon capture technologies not aimed at creating products that instead transport the carbon dioxide to storage sites for long-term storage, carbon dioxide capture and storage (CCS) (IPCC, 2018).

A central part of environmental evaluations of CCU is whether carbon dioxide emissions in the atmosphere are reduced. In carbon capture contexts, the terms CDR and NET are sometimes used. CDR stands for carbon dioxide removal and can be used when referring to technologies that (durably) store carbon originating from biogenic carbon sources or direct air capture (DAC) (IPCC, 2018). These technologies result in negative emissions, defined as "Removal of greenhouse gases (GHG) from the atmosphere" (IPCC, 2018) and are consequently also negative emissions technologies (NETs). Since the removal of carbon dioxide depends on both carbon source and storage time, not all carbon capture technologies are NETs resulting in CDR. Thus, in LCA studies of CCU, it is essential to consider the carbon source and storage time in order to assess whether carbon in the atmosphere is reduced.

CCU systems can have three possible sources of carbon, atmospheric, biogenic and fossil and different products with various uses can be produced (see Figure 2.2). An atmospheric carbon source follows its own path of DAC, while biogenic and fossil carbon both originate from inputs to an industrial process. This industrial process is the one where the flue gas is captured, and also this process produces some product or function (e.g. heat and electricity, cement, waste incineration). Generally, the captured flue gas is treated in a capture process to produce CO_2 (of purity depending on the requirements of the following use). Regardless of whether the CO_2 is captured from an industrial point source or directly from the atmosphere, the conversion step follows in a CCU system (this is where a CCS system would follow a different path). The conversion step produces a new product, using the carbon in the CO_2. As with any product, it is then used and treated at its end of life.

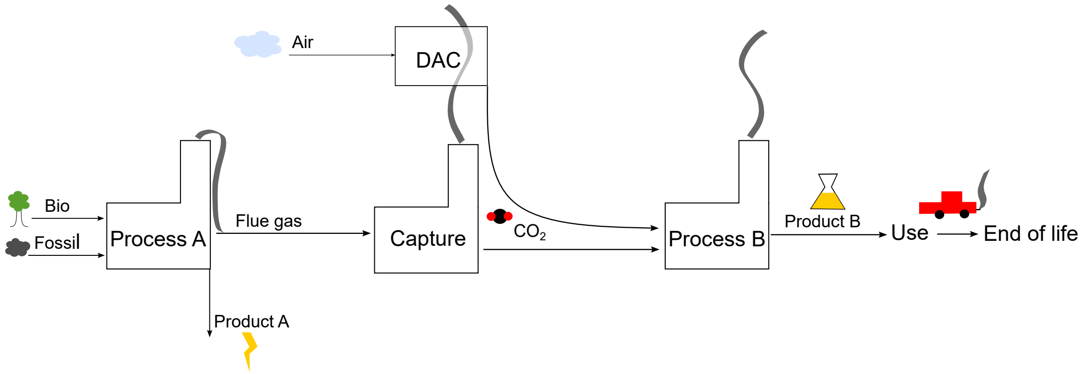

Figure 2.2: The general industrial system of a CCU system. Product B is a product that can also be delivered by another (conventional) process.

Technology development of CCU technologies

Carbon capture projects, including CCS projects, have increased recently. According to IEA (2023), the number of CCUS projects in development has increased from fewer than 100 in 2020 to around 400 by mid-2023. Considering urgent climate goals such as the Paris Agreement of limiting the temperature increase to below 2 °C above pre-industrial levels (UNFCCC, 2016), environmental evaluations of these technologies can play a role for the ongoing development. The need for LCA of CCU was discussed already by Aresta and Tommasi (1997), who highlighted the need for comparative analysis of CCU to the existing processes or products, to evaluate whether CCU reduces carbon dioxide emissions. To guide the development of CCU systems, the LCA studies need to be understandable and in line with the climate goals.

Main challenges with LCA of CCU systems

CCU systems are complex systems and it is not straightforward how to handle issues like carbon flows, multifunctionality or allocation in LCA of such systems. Several guidelines have been published specifically for LCA of CCU, e.g., Langhorst et al. (2022), Müller et al. (2020), Raadal and Modahl (2022), Ramirez et al. (2020), Skone et al. (2022), and von der Assen et al. (2013, 2014). These guidelines differ, and some recommend specific method choices when performing LCA of CCU (Langhorst et al., 2022; Müller et al., 2020;

Raadal & Modahl, 2022; Skone et al., 2022; von der Assen et al., 2013). Others give more general advice (Ramirez et al., 2020; von der Assen et al., 2014). However, this raises a question whether these guidelines are used in practice, in LCA studies of CCU systems.

Previous reviews of LCA of CCU have found methodological issues and diverging results, to which they propose harmonisation as a solution (Garcia-Garcia et al., 2021; Thonemann et al., 2022). However, the diversity of CCU technologies under development and the possible products produced from these systems implies that all LCA studies of CCU can not be the same. Given the variety of LCA studies that can be conducted for different purposes, and the diverse LCA approaches that can be used to assess emerging technologies, these studies can not and should not be directly compared.

2.3 Synthesis of background

The goal definition is the foundational step in LCA, setting the direction for the entire study. The goal and scope phase of LCA involves defining what will be assessed, for whom, and how. Better understanding the current practices in goal and scope definition in the context of CCU is important for the environmental assessments so that these inform technology development towards mitigating climate change in an effective way. This points to a need to look more closely at different types of goals and scopes and see how these align with each other. This could eventually help ensure that LCA studies address the specific needs of the commissioner and the intended application.

For emerging technologies, such as CCU technologies, LCA can guide their future development. The goals and scopes in LCA studies are particularly important for addressing knowledge needs in early technology development stages. This requires clearly defined goals with appropriately tailored scopes of the studies, ensuring that the assessments are relevant and comprehensive despite the inherent uncertainties and data limitations at early development stages.

There is thus a need to better understand what constitutes good practice in definition of goal and scope, and the different types of LCA studies supporting technology development. Studying the goals and scopes in LCAs of emerging CCU technologies, can help improve methodological guidance of LCA which in turn can improve LCA application in technology development.

CHAPTER 3

Methods

This chapter outlines the methodology used to address the research questions with the aim to improve understanding of goals and scopes in life cycle assessment (LCA) studies of carbon capture and utilisation (CCU) systems. The research design includes the different research studies, their type of data and approach for analysing their results. Lastly, limitations with the research design are discussed.

3.1 Research context

The research is performed in the context of the PYROCO$_2$ project, which has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101037009. The PYROCO$_2$ project is used as the practical case for empirical study of LCA of CCU, both for performing the analysis and also for learning about the LCA work from the LCA practitioner's perspective.

In the PYROCO$_2$ project, the conversion of carbon dioxide (CO_2) and hydrogen (H_2) into acetone through a fermentation process will be demonstrated. Using industrial CO_2 and green H_2, the project aims to produce *climate positive* acetone (PYROCO_2, 2024a). The acetone can be further upgraded into different products, chemicals, synthetic fuels and polymer materials with a *negative carbon footprint* (PYROCO_2, 2024a). The conversion process consists of a two-step thermophilic fermentation, illustrated in Figure 3.1.

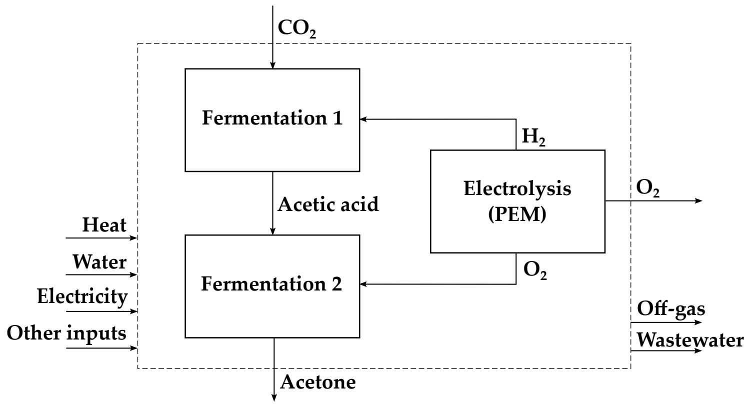

Figure 3.1: A simple flowchart of the foreground system of the studied PYROCO_2 system.

Several activities are performed within the frames of the PYROCO_2 project, for instance feedstock preparation, bioprocess development, process design and chemo-catalytic development (PYROCO_2, 2024b). The LCA work is done within the work package for process integration and sustainability assessment. Within this work package, techno-economic, environmental and social assessments will be performed. Before the LCA presented in Paper B, two master thesis projects have been conducted in the PYROCO_2 project connected to LCA of the PYROCO_2 process, by Jiresten and Larsson (2022) and Carlsson and Barclay (2023).

In the 5 year project, the technology will be developed from technology readiness level (TRL) 4-5 to TRL 7, through the engineering and building of a demonstrator plant. The demonstrator plant will be built at Herøya Industrial Park in southern Norway, but in the project several CCU hubs throughout Europe are possible future implementers of the technology. Hence, the PYROCO_2 project provides a CCU system under development, planned to be implemented in the future, that can be studied via LCA studies.

3.2 Conceptualisations

There are a few concepts that are central in my research, these are:

- **Goal definition and scope definition** becomes the way of referring to goal and scope definition to separate their respective meanings.
- **LCA types and LCA uses** are two distinct concepts. LCA types refer to LCA studies utilising different methods, thus studies with different scopes. On the other hand, LCA uses refer to the application of the LCA study or how the audience can use it, thus directly connected to the goals. Additionally, one LCA type can have multiple LCA uses, and one LCA use can be addressed by multiple LCA types.
- **Technology development** is in this licentiate thesis simplified as the technology readiness levels (TRLs) in sequence. While there are more elements to the process, these are not studied in detail.

3.3 Research design

This section outlines the research design employed to achieve the aims of this licentiate thesis, which focuses on the goals and scopes of LCA studies within the CCU domain. To address the research questions, this research employed a mixed-methods approach, involving a literature review and a case study. The literature review aims to provide insights on LCA studies of CCU, especially on the characteristics of goal and scope (RQ 1) by investigating published LCA studies. A case study is used to explore the methodology first-hand by performing an LCA of a CCU system. This aims to investigate if better attention to defining the goals and scopes in LCA studies is possible and useful, particularly in the context of a project in technology development (RQ 2). The case study is performed within the $PYROCO_2$ project, where the research has been performed.

The relationships between the papers and the research questions is visualised in Figure 3.2. The results of Paper A influenced the design of the LCA study in Paper B. While RQ 1 is connected mainly to Paper A, RQ 2 is connected to Paper B but also insights from RQ 1.

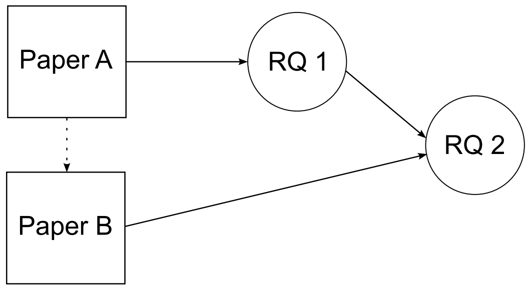

Figure 3.2: A visualisation of the relationships between the papers and the research questions (RQs).

Literature review (Paper A)

For RQ 1, a literature review was the main research method, used to gather knowledge on the goal and scope in LCA, find reviews of LCA methodology, reviews of LCA of CCU, CCU-specific LCA guidelines and centrally gather the LCA studies on CCU systems for a review of methodological practice. The literature review presented in Paper A examined the current practices in LCA of CCU, and the types of assessments conducted. It also explored the relevance and alignment of these methodologies with the aim of decarbonisation, particularly in the context of climate urgency.

A systematic search and review was the main method for data collection and analysis. The reviewed articles were found in Scopus, Web of Science and Google Scholar through searches of the concepts of life cycle assessment and carbon capture and utilisation. The collected articles were reviewed on their objects of study (sources of carbon and products created) and methodological features. The coherence between the defined goal and the scope, reported results, and handling of time aspects were also reviewed.

To identify the scopes of the models in the LCA studies, a framework was developed to locate the system boundaries of the LCA studies. Different starting points were marked in an illustration of the industrial system focused on the flow of carbon. For these starting points, a new terminology was introduced, with the three distinct "cradles" source, capture or feedstock (see Figure 3.3).

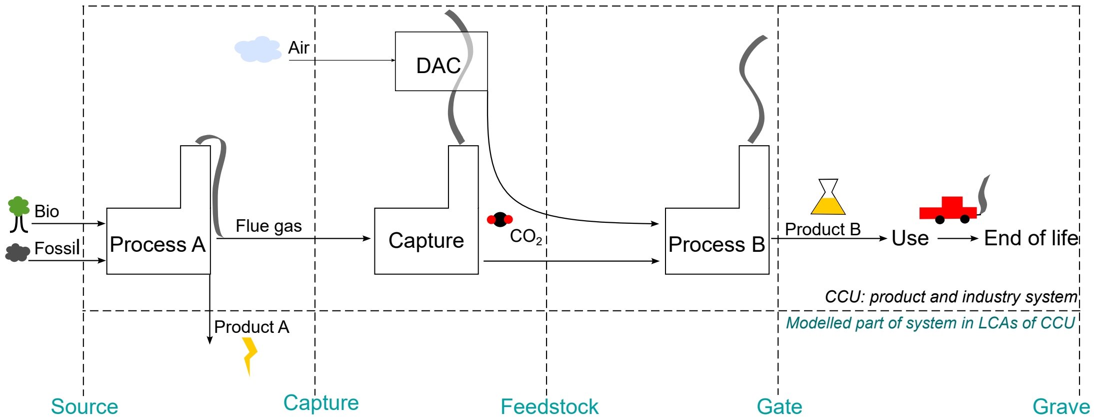

Figure 3.3: Industrial system framework with vertical lines for starting and ending points in modelling an industrial system in LCA of CCU systems.

Case study (Paper B)

To explore the importance of the goal and the scope in LCA practice first-hand, an LCA study was performed within the PYROCO$_2$ project. The LCA study was conducted with particular attention to goal definitions and their respective scope definitions following insights from Paper A. To better understand the goal and scope definition phase in LCA, goal definition and scope definition were considered separately but sequentially. Furthermore, how these goals address knowledge needs in technology development (as in relevance per TRL stage) was analysed.

The LCA study presented in Paper B was done within the frame of the EU project and results were delivered in an internal report in March 2024. The goals of the LCA study were set in collaboration with the project consortium, and results presented and discussed at project meetings.

The project consortium also provided information about the PYROCO$_2$ process. For the LCA study of acetone production from the PYROCO$_2$ process, partners in the consortium provided simulations, calculated data and assumptions on the PYROCO$_2$ process. Data was also retrieved from literature and databases (Ecoinvent) for processes not developed within the project consortium. LCA results were calculated and analysed using the tool ActivityBrowser in combination with Python and Brightway2.

3.4 Limitations

This research focuses on LCA for technology development but is limited to the field of CCU. Moreover, the case study is limited to a specific CCU system within a particular project context. Consequently, the learnings are limited to what can be explored within this single project. This is also restricted by the PYROCO$_2$ project, particularly the development of the system in the project and the partners involved in this.

Since the case study is restricted to the PYROCO$_2$ project, the exploration of LCA during technology development is limited to this particular technology development context. This might still be generalisable to similar technology development projects, but maybe not to all types of technology development projects.

This licentiate thesis is focused on issues regarding goals and scopes of LCAs. However, research conducted and presented in the included papers also concerns other subjects. For instance, the environmental impacts of CCU, in particular in the case of the fermentation process in the PYROCO$_2$ project. Furthermore, the review of published LCA studies was not solely focused on goals and scopes, but understanding LCA studies of CCU systems and thus also handled aspects like CCU-product, carbon sources, reported results and discussing the time aspect. Consequently, this licentiate thesis does not exhaustively present all the research conducted.

CHAPTER 4

Results

This chapter presents the main results and contributions from the included papers. The results cover some key features of the current methodological practice for goal and scope definition in life cycle assessment (LCA) studies of carbon capture and utilisation (CCU). The results also present initial findings on how the diversity of goals in LCA of CCU inform different knowledge needs during technology development.

4.1 LCA of CCU practice: findings from the literature

106 published LCA studies of CCU systems were found and reviewed (Paper A). It was found that CCU systems presented in the LCA articles varied greatly regarding what technologies and products were studied and the extent of the scope of the industrial system that was modelled in the LCA studies. Most common were studies that modelled the capture of fossil carbon and

conversion into C1 chemicals. For these and the others, cradle to gate was often the stated system boundary, but upon closer inspection there was a greater variation in the scope of the LCA models in these studies (see Figure 4.1). It is worth noting that there is a considerable discrepancy between the stated system boundary of the LCA models in the papers and the identified system scope of these studies. In short, the published LCA studies showed a diversity of industrial production and consumption systems within CCU systems and a diversity of LCA types.

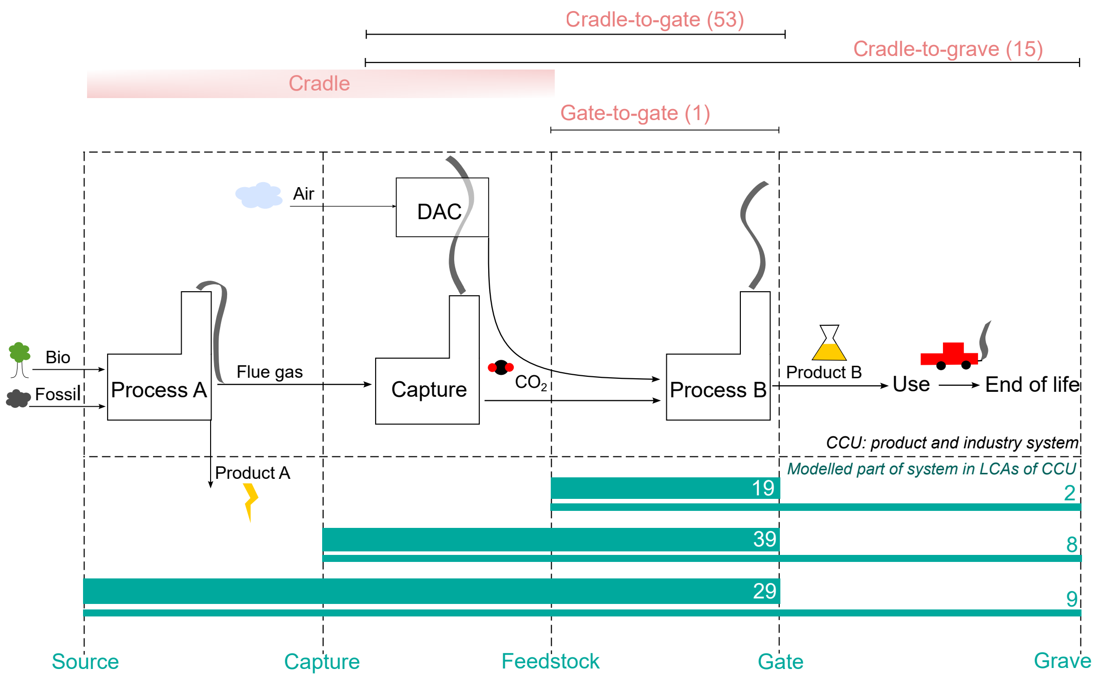

Figure 4.1: A schematic representation of the modelled part of the industrial system in the reviewed LCA studies, in relation to the industrial system. Above: stated system boundaries in the reviewed LCA studies. Below: identified boundaries with new terminology.

When looking at the stated goals for the published LCA studies, an issue of ill-defined goals was found. In half of the studies the goal of the LCA was not found and in most of the remaining studies the goal with the LCA was vague, e.g., "determine the environmental impacts" or compare a CCU product to a conventional alternative. The purpose of an LCA study or for whom the study was done was seldom identifiable in the articles. However, many studies presented different types of comparisons, either of different types of variations of a CCU system or of the CCU-based product with conventional alternatives.

The results of the reviewed LCA studies focused on climate change impact and the majority of the studies reported a reduced climate impact in favour of the studied CCU. In around a quarter of the studies, net-negative climate change impacts were reported. In contrast, only 7% of the studies reported that the studied CCU system was less favourable than the conventional alternatives.

The reviewed articles dealt with CCU systems at various stages of development, but very few of these handled or explained the time aspect at all. A handful of studies modelled a future background system (Al-Qahtani et al., 2020; Marbaix et al., 2020; Quéheille et al., 2021; Rosental et al., 2020; Rumayor et al., 2020) and a few modelled changes in the foreground system and/or scale-up of the investigated process (Cuéllar-Franca et al., 2019; Guzmán et al., 2021; Paulillo et al., 2021; Rumayor et al., 2019; Thonemann & Pizzol, 2019; Thonemann & Schulte, 2019). Only a handful of the studies discussed the time of carbon storage in the studied products, permanent or temporary (Fernández-Dacosta et al., 2019; Kashefi et al., 2020; Kätelhön et al., 2019; Ostovari et al., 2020; von der Assen et al., 2015), but did so without calculations. None of the studies indicate the point in time for construction of each CCU plant or the carbon payback time for such constructions. Given the intention of CCU for climate impact mitigation, such insufficiency of climate relevant modelling and analysis was surprising.

To better understand the LCA studies, a more detailed analysis was performed on a smaller group of studies within the reviewed articles (9 studies with the same system boundaries). From this detailed analysis it was possible to infer that a seemingly similar group of studies actually consisted of different types of LCA, i.e., studies with different goals and types of functional unit. The identified types were: studies for identifying process design improvement, studies about production route alternatives, comparison of product uses, comparison of processes cradle-to-gate and studies supporting an investment decision for the emitter.

It was also found that the reviewed LCA studies did not refer to using any of the available guidelines for method guidance. In the case of referring to any guidelines, around half of the reviewed studies cited some of the CCU-specific LCA guidelines but mainly for background information or at best, in a quarter of the reviewed studies, a specific method choice (e.g., justifying the choice of functional unit or allocation method).

Generally in the reviewed LCA studies, most method choices were described but not explained. When it came to descriptions of goal and scope definitions, the emphasis was clearly on scope definition and not on goal. This lead to difficulties to understand and interpret the results of the studies.

4.2 Case study findings

Informed by the methodological review of the LCA studies on CCU, the goal and scope was given particular attention in the LCA study performed in the PYROCO_2 project (Paper B). This was done by discussing various goals with partners in the project consortium and then articulating these for the LCA study. This resulted in three goals, but a broader purpose of providing information and learnings about the system for the PYROCO_2 consortium and external actors was also stated. The three more specific goals were about finding hotspots for technology developers, exploring locations and other variables for future implementation and comparing to conventional alternatives to inform prospective investors. These goals were elaborately stated in the report and the paper. Next, the scope corresponding to each goal was not only presented but also explained. Method choices in the scope definition were also explained, in relation to the specific goals of the LCA study. It became clear that the specific method choices for the performed LCA study were influenced by the purpose to inform and learn about the system, and were adjusted to the audience of primarily the PYROCO_2 consortium. Therefore, the scope was kept to what was relevant for the consortium at this stage in the project (at TRL 4-5) and meant to inform the further development of the PYROCO_2 process.

Regarding LCA for technology development, Paper B presents an LCA study performed within one particular technology development process. The different knowledge needs of the actors in the project were addressed by the three goals of the study. Thus, the conducted LCA study had multiple goals and fulfilled different roles within the technology development process of the $PYROCO_2$ project. It was difficult to fulfil all goals equally well with the single LCA study. This means that since there are several questions posed about the system and its future implications, there is room for more LCA studies to address the diverse knowledge needs during the technology development process further.

4.3 Summary of findings

In summary, LCA studies of CCU systems have been found to study diverse technologies, products, and use methodologies with poorly defined goals. This made it difficult to interpret the results of the reviewed LCA studies. In turn, this has implications for the interpretation of the climate impacts for CCU. The reviewed studies reported predominantly reduced climate change impacts, and some even net-negative impacts, but then without any explicit consideration of the time aspect of carbon storage.

Paper B, informed by the review in Paper A, emphasised clear goals defined. The study had three specific goals to address several knowledge needs in the technology development and the method choices and results were tailored to these. The paper also highlighted the need for multiple LCA studies to fully understand the system's future implications and support technology development.

The next chapter will analyse these findings in the context of the research questions.

CHAPTER 5

Analysis

The findings presented in Chapter 4 are analysed in relation to the research questions. The research questions concern the current methodological practice of goal and scope in life cycle assessment (LCA) studies of carbon capture and utilisation (CCU) and different goals in LCA of CCU for addressing knowledge needs during technology development.

5.1 Current practice of goal definition and scope definition in LCAs of CCU

It was found (in Paper A) that the purpose of an LCA study was rarely, or not clearly, stated in the goal definition of the reviewed LCA studies of CCU systems. Instead there was mainly a description of the defined scope in the form of key method choices. When any explanations are not given, the reader of the LCA article must develop their own interpretation of the study. The majority of the reviewed LCA studies reported favourable climate impact results, but the unclear goals and limitations in climate-relevant modelling cast doubt on the reliability of these findings. There is thus room for improving the practice of goal definition in LCA, or at least improve the reporting of it in LCA articles.

These insights on the goal definition and scope definition from the review (Paper A), affected how the LCA case study (Paper B) was performed. Because of this, more emphasis was given to the goal definition and the goals' meaning for the scope definition and representation of the LCA results. Regarding the scope, this was also affected by the results of the review of LCA studies. The same model of the industrial system as in the framework (in Paper A) was used to show which parts of the system were modelled in the LCA study (in Paper B).

The review (in Paper A) showed clearly that the scopes of modelled systems in the reviewed LCA studies differ considerably and that terminology was inconsistent. The LCA studies included different stages of the industrial system in their LCA model, often with the same system boundaries stated, e.g., "cradle-to-gate". When sorting the reviewed LCA studies according to the industrial system framework, several categories of studies were found, distinguished by modelling the "cradle" at different places in the industrial system. Nevertheless, upon closer inspection, one category of seemingly similar studies (all with the same system boundaries) consisted of very different studies. There is therefore also room for improving scope definition in LCA practice, partly to better describe the scope of the modelled system and partly to better explain (and not just state) method choices in relation to the defined goal(s).

5.2 Identifying types of LCA studies of CCU

The current practice for LCA of CCU was found (in Paper A) to be diverse in both the systems studied and the methodologies used. It became impossible to identify the types of LCA studies from reading a study's goal, since this was often not identifiable or understandable. Instead, the goal or purpose of an LCA study had to be inferred from its chosen methods and reported results. This was done for a small group of studies in Paper A which lead to the identification of five distinct types of LCA studies. These types of

LCA studies of CCU were made, for example, from the perspectives of process design, industrial production routes, product use, product cradle-to-gate comparison or investment decision whether to implement CCU in an existing system. These LCA studies with different perspectives were presumably done with specific purposes for different actors, which should be stated in the goal definition. Instead of relying on inference, clear reporting of goal(s) for an LCA study would help improve understanding of what types of LCAs exist and are applied.

It was possible to identify a few types of LCA studies from Paper A. Most likely, more types of LCA studies are possible when assessing CCU systems. Since these types identified were only inferred from studying a subset of articles in detail, some information regarding these types might be missing. This identification could only study what had been reported, not what the underlying intentions or actual situations were.

In the case study (in Paper B), the types of LCA studies of CCU was further explored through performing one LCA study and reflecting on the purposes and uses of this study. This exploration particularly focused on the types of LCA for technology development as that was the context of the case study. This resulted in further insights regarding types of LCA studies and their goals, adding to the five types already found from reviewing nine studies in detail.

5.3 Conducting LCAs of CCU for technology development

Conducting the LCA study (in Paper B) allowed for a comparison between activities performed for carrying out the study with those describing the procedural phases in LCA methodology. Two key aspects to highlight are the procedure for defining goal(s) for the LCA study and the usefulness of having an overview of the industrial system before deciding which parts of it should be included in the LCA model. These two aspects will be further elaborated on in the following.

In the case of the LCA study in Paper B, goal definition was conducted through interactions with the partners in the technology development project $PYROCO_2$. This led to the identification of thee different goals to be investigated with LCA. These three goals addressed knowledge needs in technology development in different ways. The first that focused on finding hotspots addressed knowledge needs of the technology developers considering the design of the process and configurations of the system. The second goal, that was handled by analysing scenarios of different future circumstances, reflected the need for knowledge on where and in what industrial systems a future version of the PYROCO$_2$ system could be environmentally beneficial. The third goal was about comparing the produced product to conventional alternatives, directed towards marketing of the process towards possible investors. Hence, the three goals addressed distinct knowledge needs and distinct actors in the project consortium.

The types of LCA studies identified in the review of LCA studies of CCU in Paper A can be compared to the types of goals in the LCA study in Paper B. The first goal of the LCA case study can be categorised as process design improvement and the third goal is similar to the product-focused "cradle-to-gate comparison". On the other hand, the second goal does not fit into any of the types identified in Paper A and thus adds a sixth type of LCA study: comparison of locations and circumstances. It is similar to the type "investment decision", but that is from the perspective of the emitter, which was not included in this particular study.

These types of goals, hence types of LCAs, can tentatively be placed on the technology readiness level (TRL) scale to show which stages of the technology development process they can support. This is visualised in Figure 5.1.

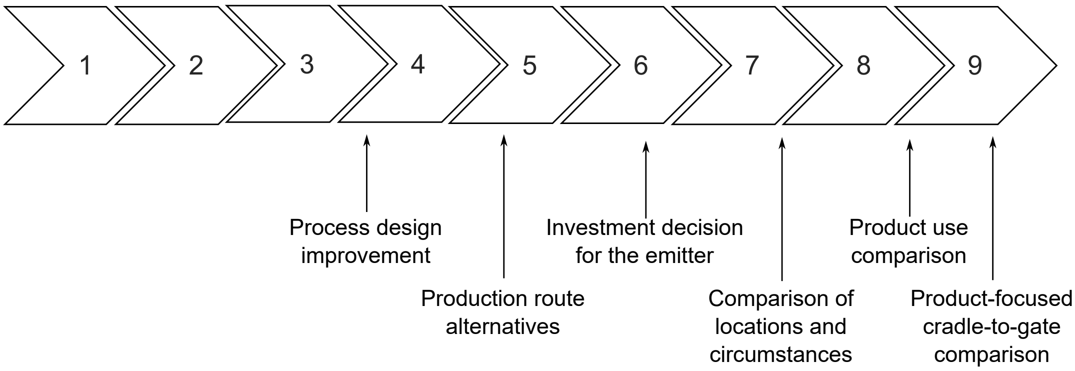

Figure 5.1: Technology readiness levels (TRLs) and the identified LCA types placed along them.

The overview of the industrial system (as illustrated in Figure 2.2, 3.3 and 4.1), was used in the PYROCO$_2$ project to describe the industrial system of CCU and the scope of the LCA study conducted. This visualisation helped identifying which processes are generally included in a CCU system and which were studied in the LCA study. Hence, it clarified which parts of the industrial CCU system were not included. During presentations within the PYROCO$_2$ project, this overview helped explain the extent and the limitations of the LCA study.

Since one LCA study with three goals could not answer all the posed questions fully, other LCA studies on the same system within the technology development are needed. These LCA studies might address different knowledge needs, have different goals and thereby different scopes. The multiple types of possible LCAs highlight the importance of contextual understanding for identifying goals in LCA of CCU, and understanding their roles in addressing knowledge needs during technology development.

CHAPTER 6

Discussion

The review in Paper A revealed that the goal definition in goal and scope definition is often missing or insufficient, in life cycle assessment (LCA) studies of carbon capture and utilisation (CCU) systems. The guidelines state that the goal definition should include the purpose of the assessment, the intended application, the intended audience and whether the results are for public comparisons (e.g., Baumann & Tillman, 2004; Curran, 2017; ISO, 2006). However, this has not been covered in the descriptions of goal and scope definitions in any of the reviewed LCA studies of CCU. The reasons for this are still unclear from the conducted research and require further investigation. However, it also raises questions about how goal definition and scope definition, respectively, are understood and handled.

The historical differences in the naming of the first phase of LCA, either as only goal definition (Guinée et al., 1993) or goal definition and scoping (Lindfors et al., 1995), in contrast to the current ISO standard where it is called goal and scope (ISO, 2006), points towards two separate methodological activities of somewhat different character. There is a difference between defining the goal and scope, or defining first the goal and then doing the scoping. The latter approach was tried in the case study in Paper B, where the goal definition and the scope definition were handled separately.

Handling goal and scope separately proved to be useful for the understanding of the LCA study and its use in technology development. A representation of this LCA procedure is given in Figure 6.1. The goals with the LCA study proved to each have different purposes and be directed towards different actors and different stages of the technology development process.

In the published LCA studies, there was an imbalance between the goal definition and the scope definition. Even though both steps are mentioned in LCA guidelines, and LCA studies transparently report what they have done, there was a heavy focus on the scope definition. Separating the goal and the scope definitions and treating them as two distinct but related activities, in guidelines and in practice, would help improve LCA practice.

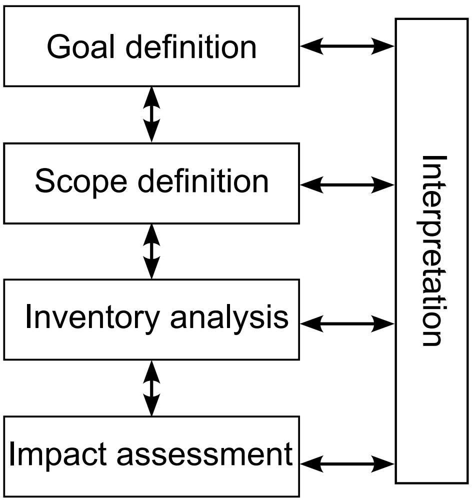

Figure 6.1: The LCA procedure of the performed LCA in Paper B.

It is known that there can be different goals and uses of LCA in different technology development stages of emerging technologies (Bergerson et al., 2020; Gavankar et al., 2014; Hetherington et al., 2013; Thomassen et al., 2019). The listed goals are typically generally formulated goals, such as the main goals with techno-economic and life cycle assessments at different technology readiness levels (TRLs) presented by Thomassen et al. (2019) or the common types of decisions being informed using LCA for emerging or mature technologies in emerging or mature markets (Bergerson et al., 2020). A common type of decision is whether or not to introduce emerging technologies into mature markets. For this, Bergerson et al. (2020) propose comparison to incumbent and hotspot analysis. This decision was also the case in the LCA study in Paper B. However, there were also other uses specific to the project such as informing choices of future locations. Moreover, these articles state that there can be different goals or uses for LCA, but do not provide guidance on how to perform such LCA studies, e.g., which method choices to make.

The identification of three different goals with the LCA study in Paper B indicates that at least three different types of LCA studies could be performed on the same system, for different purposes. This points towards performing multiple LCA studies in the same project, something that is seldom mentioned. Previous research has stated that different LCA approaches are suitable at different stages (e.g., Baumann & Tillman, 2004; Bergerson et al., 2020; Gavankar et al., 2014; Thomassen et al., 2019), but does not make clear that several of these approaches could (or even should) be applied in the same technology development process. Sandin et al. (2014), in their discussion about different roles of LCA studies in research and development projects, discussed performing a screening LCA early in a project, but still to aid the LCA later in the project. Also in the field of prospective or ex-ante LCA (e.g. Arvidsson et al., 2017; Buyle et al., 2019; Cucurachi et al., 2018; Thonemann, 2020), the discussion is on how to do the prospective LCA, as if this is the one and only way to perform LCA of emerging technologies.

To conclude, LCA is a flexible methodology and it has been previously noted that there can be different LCAs for emerging technologies. What has become clear from the present research is that there can be multiple and different LCAs within one technology development process to serve the many decisions or knowledge needs during that process. For each of these, a typical goal could be articulated and a matching scope could be developed.

CHAPTER 7

Conclusions

This research has looked into the topic of goal and scope definition in life cycle assessment (LCA) studies of carbon capture and utilisation (CCU), first through a review of published LCA studies, second through an LCA case study. The focus on goal and scope is motivated by the need to support technology development and address climate urgency effectively.

Firstly, the research indicates that treating goal definition and scope definition as separate but related activities can lead to more understandable and transparent studies. This approach was beneficial both in the review of LCA studies and the LCA case study.

Secondly, there is a need for more detailed guidance on how different types of goals should be translated into appropriate scopes. This is crucial for ensuring that LCA studies support the specific knowledge needs of CCU technology development projects.

Thirdly, the research highlights the importance of clearly defining goals to address different knowledge needs within a single CCU development project. This clarity is essential for selecting the right methodological choices and ensuring the LCA study's relevance and usefulness.

However, current LCA guidelines, including those specific to CCU, lack detailed instructions on how to link goals to methodological choices. This gap can lead to insufficiently defined goals and weak connections between goal and scope in practice. To improve this, both general and CCU-specific guidelines should provide clearer guidance on defining goals and translating them into scopes.

In conclusion, enhancing the clarity and connection between goal and scope definitions in LCA studies is important. This will help LCA practitioners define their goals in collaboration with commissioners and translate these goals into scopes that yield desired outcomes and are effectively communicated. From first-hand experience in performing an LCA of CCU during technology development, it is evident that making method choices based on specific goals is neither straightforward nor intuitive, underscoring the need for improved guidance.

7.1 Future research

More research is needed to improve guidance on different goals and what their related scopes look like, especially within technology development such as CCU systems. Conducting diverse LCA studies on the same system with varying goals can further enhance the understanding of goal and scope. This requires exploration through various types of LCA studies (on the same system) with distinct purposes. Additionally, more LCA studies on the same system can provide deeper insights into the goal and its implications by examining how the scope changes with different goals. The case study presented in this licentiate thesis can serve as a practical example for empirical investigation through multiple LCA studies.

The industrial system framework that was presented in Figure 3.3 and later used in Figure 4.1 (from Paper A) could be used when performing an LCA to map the modelled system in the industrial system. To be of more use for the LCA practitioner and the audience of the LCA results, such types of frameworks would need further development. What parts of the industrial system is included in the LCA model is one dimension of the LCA modelling but there are more dimensions which could be included in this framework. For example, the actors involved or the actor from which perspective the LCA is performed could be another dimension, to communicate the purpose of the LCA better. Furthermore, the perspective of time would ideally be represented in such a representation of an LCA study.

7.2 Recommendations to practitioners

From the research so far, treating the goal definition and scope definition as separate but related activities in the goal and scope definition phase in LCA is recommended. This allows for more emphasis on the goal definition and helps making the scope definition and LCA results appropriate to the purpose of the study. It can also improve transparent reporting of LCA studies. That said, more guidance is needed on how to make these appropriate choices as these are not explicit in the current guidelines.

Additionally, it is advisable for LCA practitioners to conduct LCA studies with various goals. Accepting different types and roles of LCA within a technology development project and carrying out multiple LCA studies can better address the knowledge needs in the project, leading to more meaningful and useful outcomes.

References

Al-Qahtani, A., González-Garay, A., Bernardi, A., Galán-Martín, A., Pozo, C., Mac Dowell, N., Chachuat, B., & Guillén-Gosálbez, G. (2020). Electricity grid decarbonisation or green methanol fuel? A life-cycle modelling and analysis of today's transportation-power nexus. *Applied Energy*, *265*, 114718. https://doi.org/10.1016/j.apenergy.2020.114718

Aresta, M., & Tommasi, I. (1997). Carbon dioxide utilisation in the chemical industry. *Energy Conversion and Management*, *38*, S373–S378. https://doi.org/10.1016/S0196-8904(96)00297-X

Arvidsson, R., Tillman, A.-M., Sandén, B. A., Janssen, M., Nordelöf, A., Kushnir, D., & Molander, S. (2017). Environmental Assessment of Emerging Technologies: Recommendations for Prospective LCA. *Journal of Industrial Ecology*, *22*(6), 1286–1294. https://doi.org/10.1111/jiec.12690

Baumann, H. (1995). *Decision making and life cycle assessment* [Licentiate thesis]. Technical Environmental Planning 1995:4. Chalmers University of Technology, Sweden.

Baumann, H., & Tillman, A.-M. (2004). *The Hitch Hiker's Guide to LCA*. Studentlitteratur AB. Lund, Sweden.

Bergerson, J. A., Brandt, A., Cresko, J., Carbajales-Dale, M., MacLean, H. L., Matthews, H. S., McCoy, S., McManus, M., Miller, S. A., Morrow, W. R., Posen, I. D., Seager, T., Skone, T., & Sleep, S. (2020). Life cycle assessment of emerging technologies: Evaluation techniques at different stages of market and technical maturity. *Journal of Industrial Ecology*, *24*(1), 11–25. https://doi.org/10.1111/jiec.12954

Bjørn, A., Laurent, A., Owsianiak, M., & Olsen, S. I. (2018). Goal definition. In M. Z. Hauschild, R. K. Rosenbaum, & S. I. Olsen (Eds.), *Life cycle assessment: Theory and practice* (pp. 67–74). https://doi.org/10.1007/978-3-319-56475-3

Buyle, M., Audenaert, A., Billen, P., Boonen, K., & Van Passel, S. (2019). The Future of Ex-Ante LCA? Lessons Learned and Practical Recommendations. *Sustainability*, *11*(19), 5456. https://doi.org/10.3390/su11195456

Carlsson, W., & Barclay, J. (2023). *Carbon flows in life cycle assessment of carbon capture: Assessing environmental impacts and carbon capture potential in industrial processes* [Master's thesis]. Chalmers University of Technology, Sweden.

Cucurachi, S., van der Giesen, C., & Guinée, J. (2018). Ex-ante LCA of Emerging Technologies. *Procedia CIRP*, *69*, 463–468. https://doi.org/10.1016/j.procir.2017.11.005

Cuéllar-Franca, R., García-Gutiérrez, P., Dimitriou, I., Elder, R. H., Allen, R. W. K., & Azapagic, A. (2019). Utilising carbon dioxide for transport fuels: The economic and environmental sustainability of different fischer-tropsch process designs. *Applied Energy*, *253*, 113560. https://doi.org/10.1016/j.apenergy.2019.113560

Curran, M. A. (2017). Overview of goal and scope definition in life cycle assessment. In M. A. Curran (Ed.), *Goal and scope definition in life cycle assessment* (pp. 1–62). Springer Netherlands. https://doi.org/10.1007/978-94-024-0855-3_1

European Commission. (2017). *Horizon 2020 Work Programme 2016 – 2017 - 20. General Annexes* (Report).

Fernández-Dacosta, C., Shen, L., Schakel, W., Ramirez, A., & Kramer, G. J. (2019). Potential and challenges of low-carbon energy options: Comparative assessment of alternative fuels for the transport sector. *Applied Energy*, *236*, 590–606. https://doi.org/10.1016/j.apenergy.2018.11.055

Garcia-Garcia, G., Fernandez, M. C., Armstrong, K., Woolass, S., & Styring, P. (2021). Analytical review of life-cycle environmental impacts of carbon capture and utilization technologies. *ChemSusChem*, *14*(4), 995–1015. https://doi.org/10.1002/cssc.202002126

Gavankar, S., Suh, S., & Keller, A. A. (2014). The role of scale and technology maturity in life cycle assessment of emerging technologies: A case study on carbon nanotubes. *Journal of Industrial Ecology*, *19*(1), 51–60. https://doi.org/10.1111/jiec.12175

Guinée, J., Udo de Haes, H., & Huppes, G. (1993). Quantitative life cycle assessment of products: 1: Goal definition and inventory. *Journal of Cleaner Production*, *1*(1), 3–13.

Guzmán, H., Salomone, F., Batuecas, E., Tommasi, T., Russo, N., Bensaid, S., & Hernández, S. (2021). How to make sustainable CO2 conversion to Methanol: Thermocatalytic versus electrocatalytic technology. *Chemical Engineering Journal*, *417*, 127973. https://doi.org/doi.org/10.1016/j.cej.2020.127973

Hetherington, A. C., Borrion, A. L., Griffiths, O. G., & McManus, M. C. (2013). Use of LCA as a development tool within early research: challenges and issues across different sectors. *The International Journal of Life Cycle Assessment*, *19*(1), 130–143. https://doi.org/10.1007/s11367-013-0627-8

IEA. (2023). *Net zero roadmap a global pathway to keep the 1.5 °c goal in reach: 2023 update* (Report).

IPCC. (2018). Annex i: Glossary [matthews, j.b.r. (ed.)] In V. Masson-Delmotte, P. Zhai, H.-O. Pörtner, D. Roberts, J. Skea, P. Shukla, A. Pirani, W. Moufouma-Okia, C. Péan, R. Pidcock, S. Connors, J. Matthews, Y. Chen, X. Zhou, M. Gomis, E. Lonnoy, T. Maycock, M. Tignor, & T. Waterfield (Eds.), *Global warming of 1.5°c. an ipcc special report on the impacts of global warming of 1.5°c above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty* (pp. 541–562). Cambridge University Press. https://doi.org/10.1017/9781009157940.008

IPCC. (2023). *Climate change 2022 - mitigation of climate change*. Cambridge University Press. https://doi.org/10.1017/9781009157926

ISO. (2006). *ISO 14040:2006: Environmental management – Life cycle assessment – Principles and framework* (Report). International Organization for Standardization.

Jiresten, E., & Larsson, O. (2022). *Life cycle assessment of acetone production from captured carbon dioxide: Using bio-fermentation at the pyroco2-pilot plant* [Master's thesis]. Chalmers University of Technology, Sweden.

Kashefi, K., Pardakhti, A., Shafiepour, M., & Hemmati, A. (2020). Ex-Situ CO2 Capture and Utilization Over the Bauxite Residue: Lifecycle and Economic Recovery Assessment. *Journal of Renewable Energy and Environment (JREE)*, *7*(4), 1–9. https://doi.org/10.30501/jree.2020.225900.1097

Kätelhön, A., Meys, R., Deutz, S., Suh, S., & Bardow, A. (2019). Climate change mitigation potential of carbon capture and utilization in the chemical industry. *Proceedings of the National Academy of Sciences*, *116*(23), 11187–11194. https://doi.org/10.1073/pnas.1821029116

Klöpffer, W. (1997). Life cycle assessment: From the beginning to the current state. *Environmental Science and Pollution Research*, *4*(4), 223–8. https://doi.org/10.1007/BF02986351

Langhorst, T., McCord, S., Zimmermann, A., Müller, L., Cremonese, L., Strunge, T., Wang, Y., Zaragoza, A. V., Wunderlich, J., Marxen, A., Armstrong, K., Buchner, G., Kätelhön, A., Bachmann, M., Sternberg, A., Michailos, S., Naims, H., Winter, B., Roskosch, D., . . . Sick, V. (2022). *Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO2 Utilization (Version 2.0)* (Report). https://doi.org/10.7302/4190

Lindfors, L.-G., Christiansen, K., Hoffman, L., Virtanen, Y., Juntilla, V., Hanssen, O.-J., Rønning, A., Ekvall, T., & Finnveden, G. (1995). *Nordic guidelines on life-cycle assessment* (Report No. Nord 1995:20).

Marbaix, J., Kerroux, P., Montastruc, L., Soulantica, K., & Chaudret, B. (2020). CO2 methanation activated by magnetic heating: life cycle assessment and perspectives for successful renewable energy storage. *The International Journal of Life Cycle Assessment*, *25*, 733–743. https://doi.org/10.1007/s11367-020-01734-8

Moni, S. M., Mahmud, R., High, K., & Carbajales-Dale, M. (2019). Life cycle assessment of emerging technologies: A review. *Journal of Industrial Ecology*, *24*(1), 52–63. https://doi.org/10.1111/jiec.12965

Müller, L., Kätelhön, A., Bachmann, M., Zimmermann, A., Sternberg, A., & Bardow, A. (2020). A guideline for life cycle assessment of carbon capture and utilization. *Frontiers in Energy Research*, *8*, 15. https://doi.org/10.3389/fenrg.2020.00015

Ostovari, H., Sternberg, A., & Bardow, A. (2020). Rock 'n' use of CO2: carbon footprint of carbon capture and utilization by mineralization. *Sustainable Energy & Fuels*, *4*(9), 4482–4496. https://doi.org/10.1039/d0se00190b

Paulillo, A., Pucciarelli, M., Grimaldi, F., & Lettieri, P. (2021). The life-cycle environmental performance of producing formate via electrochemical reduction of CO2 in ionic liquid. *Green Chemistry*, *23*(17), 6639–6651. https://doi.org/10.1039/d1gc02306c

PYROCO$_2$. (2024a). Demonstrating sustainable value creation from industrial CO2 by its thermophilic microbial conversion into acetone. https://www.pyroco2.eu/

PYROCO$_2$. (2024b). Work packages. https://www.pyroco2.eu/work-packages/

Quéheille, E., Dauvergne, M., & Ventura, A. (2021). Prospective life cycle assessment at early stage of product development: Application to nickel slag valorization into cement for the construction sector. *Frontiers in Built Environment*, *7*, 743948. https://doi.org/10.3389/fbuil.2021.743948

Raadal, H. L., & Modahl, I. S. (2022). *Guidelines for Life Cycle Assessment (LCA) of CCU systems* (Report). NORSUS.

Ramirez, A. R., Khamlichi, A. E., Markowz, G., Rettenmaier, N., Baitz, M., Jungmeier, G., & Bradley, T. (2020). *LCA4CCU: Guidelines for Life Cycle Assessment of Carbon Capture and Utilisation* (Report). the European Commission, DG ENER. https://doi.org/10.2833/161308

Rosental, M., Fröhlich, T., & Liebich, A. (2020). Life cycle assessment of carbon capture and utilization for the production of large volume organic chemicals. *Frontiers in Climate*, *2*, 586199. https://doi.org/10.3389/fclim.2020.586199

Rotolo, D., Hicks, D., & Martin, B. R. (2015). What is an emerging technology? *Research Policy*, *44*(10), 1827–1843. https://doi.org/10.1016/j.respol.2015.06.006

Rumayor, M., Dominguez-Ramos, A., & Irabien, A. (2019). Innovative alternatives to methanol manufacture: Carbon footprint assessment. *Journal of Cleaner Production*, *225*, 426–434. https://doi.org/10.1016/j.jclepro.2019.03.015

Rumayor, M., Dominguez-Ramos, A., & Irabien, A. (2020). Toward the decarbonization of hard-to-abate sectors: A case study of the soda ash production. *Acs Sustainable Chemistry & Engineering*, *8*(32), 11956–11966. https://doi.org/10.1021/acssuschemeng.0c01598

Sandin, G., Clancy, G., Heimersson, S., Peters, G. M., Svanström, M., & ten Hoeve, M. (2014). Making the most of LCA in technical inter-organisational R&D projects. *Journal of Cleaner Production*, *70*, 97–104. https://doi.org/10.1016/j.jclepro.2014.01.094

Skone, T. J., Mutchek, M., Krynock, M., Moni, S., Rai, S., Chou, J., Carlson, D., Jamieson, M., Dale, E., Cooney, G., & Kumar, A. (2022). *Carbon Dioxide Utilization Life Cycle Analysis Guidance for the U.S. DOE Office of Fossil Energy and Carbon Management Version 2.0* (Report). National Energy Technology Laboratory.

Tanzer, S. E., & Ramírez, A. (2019). When are negative emissions negative emissions? *Energy & Environmental Science*, *12*(4), 1210–1218. https://doi.org/10.1039/c8ee03338b

Thomassen, G., Van Dael, M., Van Passel, S., & You, F. (2019). How to assess the potential of emerging green technologies? towards a prospective environmental and techno-economic assessment framework. *Green Chemistry*, *21*(18), 4868–4886. https://doi.org/10.1039/c9gc02223f

Thonemann, N. (2020). Environmental impacts of CO2-based chemical production: A systematic literature review and meta-analysis. *Applied Energy*, *263*, 114599. https://doi.org/10.1016/j.apenergy.2020.114599

Thonemann, N., & Pizzol, M. (2019). Consequential life cycle assessment of carbon capture and utilization technologies within the chemical industry. *Energy & Environmental Science*, *12*(7), 2253–2263. https://doi.org/10.1039/c9ee00914k

Thonemann, N., & Schulte, A. (2019). From Laboratory to Industrial Scale: A Prospective LCA for Electrochemical Reduction of CO2 to Formic

Acid. *Environmental Science & Technology*, *53*(21), 12320–12329. https://doi.org/10.1021/acs.est.9b02944

Thonemann, N., Zacharopoulos, L., Fromme, F., & Nuhlen, J. (2022). Environmental impacts of carbon capture and utilization by mineral carbonation: A systematic literature review and meta life cycle assessment. *Journal of Cleaner Production*, *332*, 130067. https://doi.org/10.1016/j.jclepro.2021.130067

Thonemann, N., Schulte, A., & Maga, D. (2020). How to conduct prospective life cycle assessment for emerging technologies? a systematic review and methodological guidance. *Sustainability*, *12*(3), 1192. https://doi.org/10.3390/su12031192

UNFCCC. (2016). *Report of the Conference of the Parties on its twenty-first session, held in Paris from 30 November to 13 December 2015. Addendum. Part two: Action taken by the Conference of the Parties at its twenty-first session.* (Report).

von der Assen, N., Jung, J., & Bardow, A. (2013). Life-cycle assessment of carbon dioxide capture and utilization: Avoiding the pitfalls. *Energy & Environmental Science*, *6*(9), 2721–2734. https://doi.org/10.1039/c3ee41151f

von der Assen, N., Sternberg, A., Kätelhön, A., & Bardow, A. (2015). Environmental potential of carbon dioxide utilization in the polyurethane supply chain. *Faraday Discuss*, *183*, 291–307. https://doi.org/10.1039/c5fd00067j

von der Assen, N., Voll, P., Peters, M., & Bardow, A. (2014). Life cycle assessment of CO2 capture and utilization: a tutorial review. *Chemical Society Reviews*, *43*(23), 7982–94. https://doi.org/10.1039/c3cs60373c