Life cycle assessment of emerging chemical technology systems: challenges and future needs

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Chapter 3: Up-scaling methods used in ex-ante life cycle assessment of emerging technologies: a review

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Abstract

Purpose: The objective of this paper was to provide LCA practitioners with recommendations and a framework for up-scaling emerging technologies by reviewing up-scaling methods applied so far in ex-ante Life Cycle Assessment (LCA).

Methods: Web of Science was searched for articles published between 1990 and 2019 (April) using different variations of the term "ex-ante LCA" as keywords. Suitable studies were reviewed to understand the key characteristics and main methodological principles of up-scaling methods.

Results and discussion: A total of 18 studies were selected for literature review. Review results showed that most studies reported what a hypothetical up-scaled technology would look like in the future. All studies described how they estimated data; they applied different data estimation methods, using process simulation, manual calculations, molecular structure models (MSMs) and proxies. Since the review results showed that most ex-ante LCA studies followed similar up-scaling steps, we developed a framework for the up-scaling of emerging technologies in ex-ante LCA consisting of three main steps: 1) projected technology scenario definition, 2) preparation of a projected LCA flowchart and 3) projected data estimation. Finally, a decision tree was developed based on the review results that provides recommendations for LCA practitioners regarding the up-scaling procedure in ex-ante LCA.

Conclusions: Our findings can be useful for LCA practitioners aiming at up-scaling in ex-ante LCA. We provide an overview of up-scaling methods used in ex-ante LCA, introduce a framework describing the steps involved in the up-scaling process and a decision tree recommending an up-scaling procedure. The results show that in theory all data estimation methods described in this paper can be applied to estimate material flows, energy flows, and elementary flows (emissions and natural resource use). Finally, since different kinds of expertise are required for up-scaling in ex-ante LCA, we recommend that technology experts from different fields are involved in performing ex-ante LCA, e.g. technology developers, LCA practitioners, and engineers.

3.1 Introduction

The environmental assessment of emerging technologies at an early phase of their development has received increasing attention over the past few years (Wender et al. 2014). An increasing number of novel technologies are claimed to be environmentally sustainable (Pallas et al. 2018), while such claims need to be proven by carrying out, for example, early-on environmental assessments. Determining possible environmental impacts at an early stage of research and development (R&D) allows reorienting technology development towards improved environmental performance levels at relatively low costs. In contrast, changes are difficult to implement and will entail much higher costs when a technology is close to commercialization. However, this implies a change from ex-post to ex-ante environmental assessments (Cucurachi et al. 2018).

Life Cycle Assessment (LCA) has been widely recognized as a valuable framework for the assessment of technologies (Hellweg and Milà i Canals 2014). Typically, LCA is carried out for existing industrial-scale technologies, for which industrial-scale data is readily available. Application of such ex-post LCA to new technologies is problematic since their system specifications at the industrial scale are highly uncertain and large-scale process data is generally lacking. To fill this gap, ex-ante LCA has evolved in recent years, aiming to assess emerging technologies at an early stage of development by exploring, among others, possible scenarios of their future industrial-scale implementation (Cucurachi et al. 2018).

This review paper focuses on studies that performed ex-ante LCA. Van der Giesen et al. (2020) define ex-ante LCA as "performing an environmental life cycle assessment of a new technology before it is commercially implemented in order to guide R&D decisions to make this new technology environmentally competitive as compared to the incumbent technology mix". They argue that the differences between ex-ante and ex-post LCA are not so much in the general framework of LCA, but rather in the implementation of selected phases and steps, including the definition of the intended application of emerging technologies, the definition of the functional unit, the drafting of the flowchart, the estimation of future projection of the technology, related data, etc. A key property of this implementation, is the 'unknown' that ex-ante assessments have to deal with: partly or fully unknown applications, systems, flowchart, and data.

Various LCA modes exist (Guinée et al. 2018) and several of them have been used to assess new technology systems, including prospective LCA, ex-ante or anticipatory LCA, dynamic LCA and consequential LCA. The differences between these modes have already been extensively discussed (Cucurachi et al. (2018), Buyle et al. (2019), Van der Giesen et al. (2020), Guinée et al. 2018), and are outside the scope of this article. We here only focus on the ex-ante and anticipatory modes of LCA since only these specifically focus on dealing with the 'unknowns' of emerging technology systems in our view. From here onwards, we will refer to them as 'ex-ante LCA' studies.

Ex-ante LCA of emerging technologies is associated with various challenges, such as a clear definition of the function of a future system, uncertainties, and the up-scaling of the LCA data (Hetherington et al. 2014). Furthermore, both the foreground as well as the background systems in Life Cycle Inventory (LCI) databases may have to be modified to obtain a meaningful representation of the emerging technology in its future context (Arvidsson et al. 2018). Our paper particularly focuses on the challenge of up-scaling the novel and unknown part of an emerging technology in the foreground system for ex-ante LCA.

An important aspect when discussing up-scaling of technologies is a technology's TRL (Technology Readiness Level). The TRL is a method for assessing a technology's maturity, ranging from level 1, observation of basic principles, to level 9, the fully evolved operational system (Mankins 1995; Gavankar et al. 2015). The European Association of Research and Technology (EARTO) (2014) linked TRL to manufacturability (Figure 3.1).

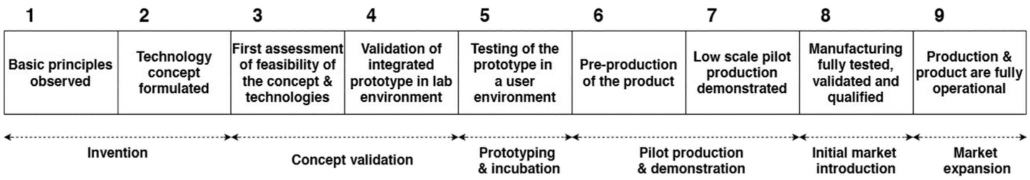

Figure 3.1 *European Association of Research and Technology (EARTO) reading on the TRL scales (source: EARTO 2014).*

In ex-ante LCA, the system specifications and data of new technologies often originate from laboratory (lab-scale) implementations (Figure 3.1: TRL 3-5) or from pilot-plant (pilot-scale) implementations (Figure 3.1: TRL 6-8). The data derived from these early realizations of a technology (lab-scale, pilot-scale) can generally not be used in the assessment of the future technology as it is far from representative of industrial-scale data (Figure 3.1: TRL 9). Industrial-scale processes may significantly differ from lab-scale and pilot-scale processes regarding the equipment and technologies used and regarding performance data (Piccinno et al. 2018; González-García et al. 2018 a,b; Salas et al. 2018). In particular, the industrial processes are generally much more efficient than the laboratory-scale or pilot-scale processes due to the implementation of complex equipment and sophisticated features, e.g. heat recovery systems and waste recycling loops. To perform meaningful LCAs on emerging technologies, the lack of industrial-scale data can be resolved by up-scaling the lab-scale or pilot-scale systems and data to projected industrial-scale levels, with or without using explicit methods and/ or scenarios.

Up-scaling in ex-ante LCA has not been extensively explored in literature so far, although various up-scaling methods have been used in ex-ante LCA studies. Some studies developed frameworks and systematic procedures for up-scaling. For instance, Shibasaki et al. (2006) introduced a systematic approach for up-scaling pilot-plant processes to industrial-plant processes. In their work, they presented technical aspects which should be considered in the up-scaling process. Piccinno et al. (2016) proposed a framework for up-scaling common processes in wet chemistry from lab scale to industrial scale. This framework comprises calculation procedures and qualitative guidance for up-scaling based on literature and expert consultation. Simon et al. (2016) introduced a framework for the estimation of industrial process data based on the results of laboratory experiments. In order to demonstrate how the framework works, the authors applied this framework to up-scale nanofiber electrospinning for Li-ion battery cathode applications. Finally, a few studies conducted a review on LCA of emerging technologies and touched upon the topic of up-scaling in LCA (Buyle et al. 2019; Moni et al. 2020; Thonemann et al. 2020).

However, little research has been done on the differences and similarities between the key characteristics and methodological principles of up-scaling methods for emerging technologies. To fill this research gap, we conducted a review of ex-ante LCA studies applying up-scaling methods. The objectives of our work were to develop a framework describing the up-scaling steps based on the review results, and to provide recommendations for LCA practitioners regarding an up-scaling procedure. With our review, we aimed to answer the following research questions:

1. Which up-scaling methods have already been applied in ex-ante LCA, and what are their key characteristics and methodological principles?
2. What steps are involved in the up-scaling of emerging technologies in ex-ante LCA?
3. Which recommendations can be given to practitioners of ex-ante LCA regarding up-scaling?

3.2 Methods

3.2.1 Literature selection

To answer the research questions, a literature search and review was done using Web of Science for studies published from 1990 to 2019 (April). Different variations of the term 'ex-ante LCA' were used as keywords: TOPIC: ("anticipatory life cycle assessment") OR TOPIC: ("anticipatory life cycle analysis") OR TOPIC: ("anticipatory LCA") OR TOPIC: ("prospective life cycle assessment") OR TOPIC: ("prospective life cycle analysis") OR TOPIC: ("prospective LCA") OR TOPIC: ("ex-ante life cycle assessment") OR TOPIC: ("ex-ante life cycle analysis") OR TOPIC: ("ex-ante LCA") OR TOPIC: ("life cycle assessment" AND "up scal*") OR TOPIC: ("life cycle analysis" AND "up scal*") OR TOPIC: (LCA AND "up scal*") OR TOPIC: ("life cycle assessment" AND "scal* up") OR TOPIC: ("life cycle analysis" AND "scal* up") OR TOPIC: (LCA AND "scal* up"). These keywords were searched in the titles, the abstracts, and the author keywords of the articles. The titles and the abstracts of publications found with these keywords were screened and studies meeting the following exclusion criteria were excluded:

- Studies that did not perform LCA;
- Review papers;
- LCA studies that developed scenarios for future development of an existing technology but did not up-scale a technology;
- Studies that performed laboratory LCA but did not perform up-scaling;

- LCA studies that up-scaled LCIA (Life Cycle Impact Assessment) results only without explicit up-scaling of inventory processes and process data;
- Ex-ante LCA studies that did not clearly describe the up-scaling procedure applied in a case study or did not describe such a procedure at all.

Studies meeting all criteria were further reviewed.

3.2.2 Literature review

We defined the two sets of criteria and reviewed all the included studies against these criteria to obtain a better understanding of the up-scaling methods applied:

1. Criteria identifying the key characteristics of up-scaling methods:
    a. What *technology* was up-scaled?
    b. What was the *starting scale* and *to which scale* was a technology up-scaled? Here we will group the studies applying up-scaling into 4 categories:
        i. from lab scale to pilot scale
        ii. from lab scale to industrial scale
        iii. from pilot scale to industrial scale
        iv. from lab and pilot scales to industrial scale
    c. Did the up-scaling method provide *results* for energy flows, material flows and elementary flows (emissions and natural resource use), or only for one or two of these?
2. Criteria identifying the main methodological principles of up-scaling methods:
    a. Was a hypothetical up-scaled technology described?
    b. Were up-scaling methods based on different estimation or calculation principles?
    c. What data was required for the applied up-scaling methods?

In section 3.4 “Discussion” we introduced a framework describing the up-scaling steps in ex-ante LCA. In addition, we discussed to what extent the included ex-ante LCA studies explicitly dealt with the steps introduced in the framework. Finally, based on the review results we developed a decision tree that provides recommendations for LCA practitioners regarding up-scaling for ex-ante LCA.

3.3 Results

Of 184 studies identified initially (Online Recourse 2), screening resulted in 18 studies that met all the criteria. In order to answer research question 1, *"Which up-scaling methods have already been applied in ex-ante LCA, and what are their key characteristics and methodological principles?"*, up-scaling methods used in the included ex-ante LCA studies were reviewed using the two sets of criteria defined in section 3.2.2 "Literature review": 1) criteria identifying the key characteristics of up-scaling methods and 2) criteria identifying the main methodological principles of up-scaling methods. Section 3.3.1 presents the key characteristics of the applied up-scaling methods and section 3.3.2 shows the results for their methodological principles.

3.3.1 Key characteristics of up-scaling methods

Table 3.1 shows the key characteristics of up-scaling methods applied in 18 ex-ante LCA studies. To be more specific, Table 3.1 describes the kind of technology that each study up-scaled, the starting and end scales for the up-scaling, and the results that were calculated after up-scaling (energy inputs and/ or outputs, material inputs and/ or outputs, and elementary flows (emissions and natural resource use)).

Table 3.1 *Key characteristics of up-scaling methods applied in ex-ante LCA.*

Study	Technology	Up-scaled from → to	Results		
			Energy inputs and/ or outputs	Material inputs and/ or outputs	Elementary flows[a]
Arvidsson and Molander (2017)	Epitaxial graphene production	Lab and pilot → industrial	✓[b]	✓	-[c]
Cossutta et al. (2017)	Graphene production	Lab → industrial	✓	✓	✓

Cuéllar-Franca et al. (2016)	Production of ionic liquids for CO_2 capture	Lab → industrial	✓	✓	-
Fernández-Dacosta et al. (2015)	Production of microbial community-based polyhydroxyalkanoates (PHAs) from wastewater	Lab and pilot → industrial	✓	✓	✓
González-García et al. (2018a)	Production of bio-succinic acid from apple pomace	Lab → industrial	✓	✓	✓
González-García et al. (2018b)	Bio-ethanol and xylooligosaccharides joint production	Lab → industrial	✓	✓	✓
Mattick et al. (2015)	*In vitro* biomass production for cultured meat	Lab → industrial	✓	✓	✓
Mazzoni et al. (2019)	Catalytic Biorefining of Ethanol from Wine Waste	Lab → industrial	✓	✓	✓
Muñoz et al. (2019)	Solar-assisted heat pump (SHP) and waste water treatment	Pilot → industrial	✓	✓	✓
Piccinno et al. (2016)[d]	Heated liquid phase batch reactions and certain isolation, purification and processing steps	Lab → industrial	✓	✓	✓
Piccinno et al. (2018)	Nanocellulose production using carrot waste	Lab → industrial	✓	✓	✓
Rinaldi et al. (2015)	Pyrolysis gasification of automotive shredder residue	Pilot → industrial	✓	✓	✓
Salas et al. (2018)	Production of geopolymer concrete	Lab → industrial	✓	✓	-

Khojasteh Salkuyeh et al. (2017)	Hydrogen production from natural gas: Syngas chemical looping (SCL) and chemical looping reforming (CLR)	Not mentioned →industrial	✓	✓	✓
Sampaio et al. (2017)	Gelatin production from tilapia residues	Lab → pilot	✓	✓	✓
Schulze et al. (2018)	Rare Earth Extraction from NdFeB Magnet Scrap Using Molten Salt Electrolysis	Lab → industrial	✓	✓	-
Simon et al. (2016)	Production of nanofibers for lithium iron phosphate cathode applications	Lab → industrial	✓	✓	✓
Villares et al. (2016)	Metal recovery from e-waste using bioleaching	Lab → pilot	✓	✓	✓

[a] *elementary flows = emissions and natural resource use (land use was not included in the review criteria);*

[b] *"✓" indicates that a study reported on the estimation of energy inputs and/ or outputs, material inputs and/ or outputs, and elementary flows;*

[c] *"-" indicates that a study did not report on the estimation of energy inputs and/ or outputs, material inputs and/ or outputs, and elementary flows;*

[d] *the authors presented an up-scaling framework for chemical processes and applied the up-scaling framework to a fictional example of a technology.*

The review results showed that studies up-scaled different kinds of technologies from different application domains, such as chemistry, waste treatment, energy, food, and the building sector (Table 3.1 and Appendix C). Most studies up-scaled chemical and waste treatment technologies (15 out of 18 studies) (Table 3.1 and Appendix C).

In general, most studies (11 out of 18) up-scaled technologies from the lab to industrial scale (Table 3.1). All studies estimated energy and material inputs and outputs, but some studies did not report how they estimated elementary flows (natural resource use and/ or emissions) (Table 3.1).

3.3.2 Methodological principles of up-scaling methods

Two studies mentioned that LCA experts had discussions with technology experts about what the hypothetical up-scaled technologies would look like (Villares et al. 2016; Schulze et al. 2018). Muñoz et al. (2019) developed a scenario of a hypothetical up-scaled technology as follows (*pers. comm.*): first, the LCA expert and the technology expert explored how the pilot-scale technology would differ from the up-scaled industrial-scale technology. Then, they determined how the pilot-scale processes should be modified, and by modifying the processes one by one, they concluded what the new technology could look like in the future in an up-scaled form.

In 5 out of 18 studies, simulation software was used to obtain a process design of a hypothetical up-scaled technology (Cossutta et al. 2017; Fernández-Dacosta et al. 2015; Mazzoni et al. 2019; Rinaldi et al. 2015; Khojasteh Salkuyeh et al. 2017). In 5 out of 18 studies, a simple conceptual process diagram was used to describe the process steps and equipment included in the hypothetical up-scaled technology (González-García et al. 2018b; Muñoz et al. 2019; Piccinno et al. 2016; Piccinno et al. 2018; Simon et al. 2016). In 1 study (González-García et al. 2018a), a simple conceptual process diagram was used as well as simulation software for the specific design of equipment.

In 17 out of 18 studies, the authors provided a description of how they viewed the hypothetical up-scaled technology, e.g. by describing assumptions about the up-scaled technology and/ or by describing the parts or processes of a new technology (Appendix C).

In 9 out of 18 studies, the authors presented a full LCA flowchart of a hypothetical up-scaled technology (Appendix C). González-García et al. (2018a, b) showed how the conceptual process diagrams of the up-scaled technology were converted to the LCA flowcharts. Other studies did not provide information on how the LCA flowchart was developed based on the simulation process design or conceptual process diagram.

All studies reported that they estimated data for each of the unit process defined in the LCA flowchart or in the simple conceptual process diagram. The review results revealed that data estimation methods used in the ex-ante

LCA studies were similar to the data estimation methods applied in ex-post LCA studies (Parvatker and Eckelman 2019):

1. Process simulation
2. Manual calculations
3. Molecular Structure Models (MSMs)
4. Use of proxy

The data estimation methods used in the included ex-ante LCA studies were classified using the classification of data estimation methods introduced by Parvatker and Eckelman (2019). The included ex-ante LCA studies estimated data for the separate unit processes defined in the LCA flowchart or simple process diagram and used a mix of data estimations methods in the up-scaling of a new technology.

Process simulation includes all data estimation methods that involve the use of simulation software and databases. The review results show that 6 of 18 included studies performed process simulation using simulation software (Cossutta et al. 2017; Fernández-Dacosta et al. 2015; González-García et al. 2018a; Mazzoni et al. 2019; Rinaldi et al. 2015; Khojasteh Salkuyeh et al. 2017). They used lab-scale or pilot-scale operation parameters as inputs for the simulation software. Energy flows, material flows and elementary flows were obtained as a result of calculations done with process simulation.

Manual calculations include all calculations done manually with the help of mathematical and physical equations, stoichiometric relationships, scaling factors, etc. Most studies (10 out of 18) performed manual calculations, although these were based on different calculation principles. For example, Piccinno et al. (2016, 2018) used basic mathematical and physical equations to calculate energy flows, material flows, and emissions. Some studies used stoichiometric calculations (e.g. Cuéllar-Franca et al. 2016) to estimate material inputs and outputs and emissions, while other studies used linear scaling of lab data to estimate material flows and elementary flows at larger scales (Piccinno et al. 2016; Sampaio et al. 2017).

Molecular Structure Models (MSMs) are models that are based on neural networks (Hornik et al. 1989) and can be used to calculate key LCI parameters and impact results using the molecular structure of a chemical (Wernet et al.

2009). One of the 18 included studies used MSMs for data estimation (Mazzoni et al. 2019). MSMs were used to estimate resource consumption and environmental impacts of the catalyst production.

Proxies can be used to approximate data by using information from a similar already existing technology that shows high resemblance with the new technology. In this review, proxy refers to an existing technology that most closely resembles the hypothetical up-scaled technology. Proxies were used for data estimation in 7 out of 18 studies (Mattick et al. 2015; Simon et al. 2016; Villares et al. 2016 ; Sampaio et al. 2017; Salas et al. 2018; Schulze et al. 2018; Muñoz et al. 2019). They retrieved proxy data from various sources, such as LCI databases (Muñoz et al. 2019; Villares et al. 2016), the literature and engineering case studies (Schulze et al. 2018; Villares et al. 2016), online catalogues of the machines (Sampaio et al. 2017; Salas et al. 2018) and expert consultation provided by technology developers (Simon et al. 2016). Energy flows, material flows and elementary flows of the new technologies were approximated by using data of a similar existing technology.

Table 3.2 shows the review results of data estimation in the ex-ante LCA studies. In Table 3.2, the columns 'Energy inputs and/ or outputs', 'Material inputs and/ or outputs' and 'Elementary flows' (under 'Data estimation') show the methods which the studies used to estimate energy flows, material flows and elementary flows, the estimation or calculation principles of those methods and the data which were used for the data estimation (see details in Appendix B). It should be noted that the studies did not estimate data for a new technology as a whole but for its separate unit processes. That is why the table shows that some studies used a mix of data estimation methods to estimate energy flows, material flows or elementary flows.

Table 3.2 *Data estimation methods used in up-scaling methods applied in ex-ante LCA.*

	Data estimation		
	Energy inputs and/ or outputs	**Material inputs and/ or outputs**	**Elementary flows***
Arvidsson and Molander (2017)	**M*:** Manual calculations **P&D*:** Calculations using thermodynamic equations; Linear scaling: assumption that electricity consumption at pilot scale is the same as at industrial scale (worst-case scenario)	**M:** 1) Manual calculations **P&D:** 1) Assumption on possible industrial parameters (expert opinion) and their use in calculations	Not reported[a]
Cossutta et al. (2017)	**M:** Process simulation[b] **P&D:** The use of the process simulation results for data estimation		
Cuéllar-Franca et al. (2016)	**M:** Manual calculations **P&D:** Calculations using the heat of formation of reactants and products and then multiplying by empirical factors (from literature)	**M:** Manual calculations **P&D:** Stoichiometry and the use of conversion yields (from literature)	Not reported
Fernández-Dacosta et al. (2015)	**M:** Process simulation[b] **P&D:** The use of the process simulation results for data estimation		
González-García et al. (2018a)	**M:** 1) Manual calculations 2) Process simulation[b] **P&D:** 1) Use of thermodynamic equations, average values and estimations (expert opinion, literature) 2) The use of the process simulation results for data estimation		
González-García et al. (2018b)	**M:** Manual calculations **P&D:** Use of thermodynamic equations, average values and estimations (expert opinion, literature)		
Mattick et al. (2015)	**M:** Use of proxy **P&D:** Calculations using operating parameters of a similar existing technology		
Mazzoni et al. (2019)	**M:** Process simulation[b]		**M:** 1) Process simulation[b] 2)

	P&D: The use of the process simulation results for data estimation		Molecular Structure Models **P&D:** 1) The use of the process simulation results for data estimation 2) Use of FineChem tool (ETH Zurich n.d.)
Muñoz et al. (2019)	**M:** 1) Use of proxy 2) Manual calculations **P&D:** 1) Assumption that electricity consumption is the same as that of a similar industrial plant 2) Calculations using experimental small-scale (pilot-plant) data	**M:** 1) Use of proxy 2) Manual calculations **P&D:** 1) Assumption of possible industrial parameters (from literature) and their use in calculations 2) Mass balance calculations based on stoichiometry and empirical relationships of parameters	**M:** Manual calculations **P&D:** Mass balance calculations based on stoichiometry and empirical relationships of parameters
Piccinno et al. (2016)	**M:** Manual calculations **P&D:** Use of thermodynamic equations, scaling factors, average values and estimations (expert opinion, literature)		
Piccinno et al. (2018)	**M:** Manual calculations **P&D:** Use of thermodynamic equations, average values and estimations (expert opinion, literature)		
Rinaldi et al. (2015)	**M:** Process simulation[b] **P&D:** The use of the process simulation results for data estimation		
Salas et al. (2018)	**M:** 1) Use of proxy 2) Manual calculations **P&D:** 1) Calculations using technical specifications for machine	**M:** Manual calculations **P&D:** Calculations using experimental lab data	Not reported

	2) Calculations using thermodynamic equations		
Khojasteh Salkuyeh et al. (2017)	**M:** Process simulation[b] **P&D:** The use of the process simulation results for data estimation		
Sampaio et al. (2017)	**M:** Use of proxy **P&D:** Calculations using technical specifications for machine (from online catalogues)	**M:** Manual calculations **P&D:** Linear scaling: assumption that the amount of reagents increases linearly from the laboratory scale to the pilot scale	**M:** Manual calculations **P&D:** Linear scaling: assumption that the amount of effluent loads increases linearly from the laboratory scale to the pilot scale
Schulze et al. (2018)	**M:** Use of proxy **P&D:** 1) Assumption that electricity use is the same as that of a similar technology (from literature)	**M:** Use of proxy **P&D:** Assumption that material inputs are the same as those of a similar technology (from literature)	Not reported
Simon et al. (2016)	**M:** Use of proxy **P&D:** Calculations using technical specifications for machine (from machine developers)	**M:** Manual calculations **P&D:** Calculations using experimental lab data	**M:** Use of proxy **P&D:** Use of emissions data (from literature)
Villares et al. (2016)	**M:** Use of proxy **P&D:** Use of adapted ecoinvent processes; Calculations using operating parameters of a similar existing technology (from engineering case study)	**M:** Use of proxy **P&D:** Assumption that material inputs are the same as those of a similar existing technology (from engineering case study)	**M:** Use of proxy **P&D:** 1) Use of ecoinvent processes; Assumption that resource inputs are the

			same as those of a similar existing technology (from engineering case study).

**Elementary flows = emissions and natural resource use, M = method, P&D = calculation/ estimation principle and data used in data estimation;* [a] *The authors expect that there will be no emissions from the up-scaled processes;* [b] *The name of the simulation software used in the LCA study can be found in Table 1 in Appendix B.*

3.4 Discussion

Assessment of emerging technologies at an early stage of R&D is crucial, as it allows for reorienting technology development towards decreased environmental burdens at lower costs. Ex-ante LCA is a tool that has emerged recently and started to be widely used by LCA practitioners in the assessment of novel technologies. While existing technologies, for which data is readily available, are commonly assessed with ex-post LCA, application of ex-post LCA to emerging technologies is challenging, as the future environmental impacts of such technologies need to be assessed when the technologies are still at the lab or pilot scale, and hence system specifications and data at industrial scale are not yet available. In order to overcome these challenges, up-scaling of technologies can be performed in ex-ante LCA. In this paper, we reviewed the differences and similarities between the key characteristics and methodological principles of up-scaling methods applied so far in ex-ante LCA.

3.4.1 A framework describing the steps involved in the up-scaling of emerging technologies

The review results show that most of the included studies followed similar up-scaling steps. Based on these results, we developed a framework that aims to distinguish between the steps of up-scaling that are predominantly based on technology expertise and the steps that are predominantly based on LCA knowledge. The resulting framework is applicable for up-scaling of technologies in different application domains. Below, we give a brief overview of technology development and ex-ante LCA, and then we introduce a framework for up-scaling a new technology in ex-ante LCA.

To the best of our knowledge, the term ‘up-scaling method’ has not yet been defined in the field of ex-ante LCA in literature. Therefore, we drafted a definition for ‘up-scaling method’ and present it below in section 3.4.1.2 “Up-scaling framework”.

3.4.1.1 Technology development and ex-ante LCA

Technology development starts with the concept development of the idea for a novel technology (TRL 1-2). In this process, technology experts may generate several scenarios. Before being able to develop an LCA model of an emerging technology system, we need to know how that system will look like in future. As technology developers are the experts in projecting scenarios of such future systems, they are the first ones to be consulted. Their scenarios particularly focus on how the specific elements of the emerging technology are expected to develop in future. The scenarios are a projection of what the technology experts expect that a technology at a low TRL will look like at a given higher TRL in future. We will refer to this as “projected technology scenarios”. We use the plural (‘scenarios’) form deliberately, because future projections of the technology represent explorations of possible futures rather than a prediction of one particular future. Next, the technology experts select a couple of scenarios that seem to be the most promising and feasible among other scenarios and develop laboratory set-ups for these scenarios (TRL 3-5). Next, the technology experts theoretically up-scale the novel technology system in one or more promising scenarios to higher TRLs (TRL 6-9). In some cases, technology experts may build pilot-scale technology (TRL 6-8) and then theoretically up-scale it to industrial scale.

Ex-ante LCA studies lacking the involvement of technology experts are of limited value unless the LCA expert is also a recognized technology expert. The latter is possible although rarely the case. Note that our view on the role of technology experts is founded on our definition of ex-ante LCA as provided in the Introduction of this article.

3.4.1.2 Up-scaling framework

Based on the review results we developed a framework for the up-scaling of emerging technologies in ex-ante LCA. This framework is comprised of three main steps: 1) projected technology scenario definition, 2) preparation of a projected LCA flowchart and 3) projected data estimation. We distinguished between projected technology scenario definition, preparation of a projected LCA flowchart and projected data estimation because we consider them to be three separate steps in the up-scaling, as they involve different types of expertise, decisions, choices and assumptions. Figure 3.2 shows a schematic representation of the framework.

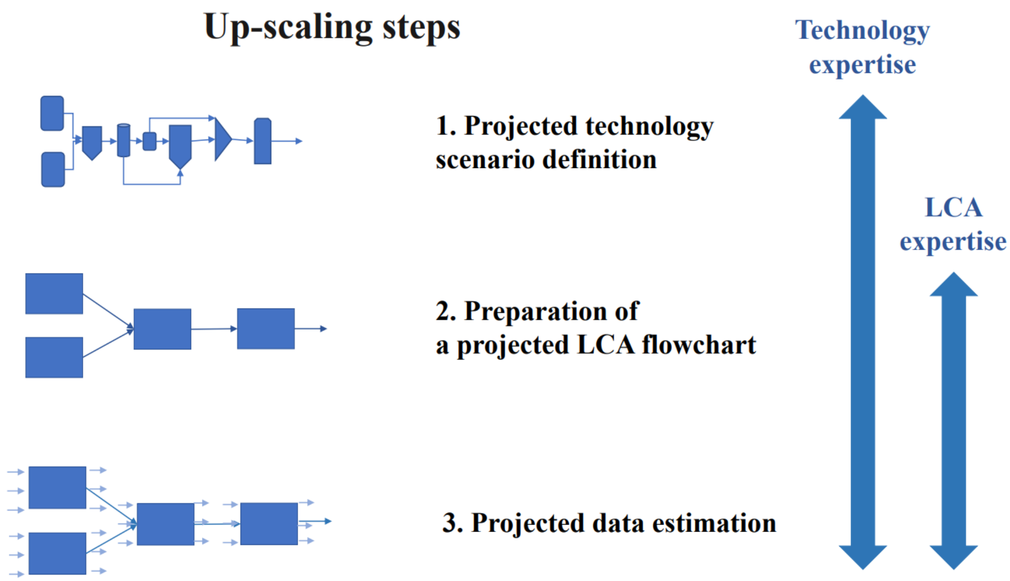

Figure 3.2 *The framework showing the up-scaling steps in ex-ante LCA.*

Projected technology scenario definition

The first step typically requires technology expertise and not so much LCA knowledge. A technology expert develops a scenario of what a hypothetical up-scaled technology may look like in the future. The expert has to decide on required process operation conditions and installations for the hypothetical up-scaled technology and can design a process flow diagram.

Preparation of a projected LCA flowchart

The next step mostly involves LCA expert knowledge. The results of the first step are handed over to the LCA practitioner. The LCA expert develops an LCA flowchart (involving a technology expert) by, for example, aggregating installations into unit processes, defining function, functional unit, reference flow, system boundaries, unit processes, etc.

Projected data estimation

Finally, data need to be estimated for the unit processes defined in the LCA flowchart by using data estimation methods. Typically, data estimation is performed by an LCA expert, but also involves technology experts, e.g. for applying process simulation software and for double checking assumptions and final data. The data estimation step is performed in iteration with the second step, ‘Preparation of a projected LCA flowchart’.

In summary, we define *an up-scaling method* as a procedure that projects how a new technology currently available at a lower TRL may look and function at a higher TRL; up-scaling should ideally be performed in three steps: 1) projected technology scenario definition, 2) preparation of a projected LCA flowchart and 3) projected data estimation.

3.4.2 Application of the framework in the reviewed studies

This section discusses whether reviewed ex-ante LCA studies followed the steps defined in the framework. The review results showed that most studies (17 out of 18) performed technology scenario definition (the first step of the framework) (Appendix C). In one study, the ‘technology scenario definition’ step was not explicitly addressed (Cuéllar-Franca et al. 2016). It is unclear whether the study defined a technology scenario: maybe the authors implicitly defined a technology scenario but did not report on that or skipped the technology scenario definition step.

In 15 out of 18 studies, it remained unclear whether technology experts were involved in the technology scenario definition or not. We assume that some studies involved technology experts in the up-scaling process without mentioning it, since the studies used simulation software and made assumptions on the process operation parameters, which requires knowledge of technology and engineering. We recommend that technology experts be involved in the technology scenario definition step and that the studies report on how they defined a technology scenario, i.e. describe how they came up with the scenario, and describe the process operation conditions and installations they defined for an up-scaled technology.

It appeared that 50% of the studies did not design full LCA flowcharts (9 out of 18). Some studies prepared simplified process diagrams and used those diagrams for the data estimation step. We recommend that LCA experts prepare full LCA flowcharts and present those as part of their reporting to be transparent on assumptions and on the translation of technology expert scenarios into LCA flowcharts.

The review results showed that the data estimation methods used in ex-ante LCA were similar to the data estimation methods applied in ex-post LCA: plant data, process simulation, manual calculations, MSMs, and using proxy.

Ex-ante LCA studies in the present review estimated data for a separate unit process of the LCA flowchart or simple process diagram and used a mix of data estimations methods in the up-scaling of a new technology. Data estimation was mostly performed using manual calculations (10 out of 18 studies). This could be due to the fact that most studies assessed chemical technologies and the data (equations specifically derived for chemical processes and the data of process operation conditions) were readily available for manual calculations. Process simulation was used in a smaller number of studies than manual calculations (6 out of 18 studies). The reason could be that process simulation is more challenging than manual calculation. For example, process simulation requires more comprehensive data (more detailed data of process operation conditions) than manual calculations, and, in addition, it requires access to simulation software, expertise in process design and skills in software use. In 7 out of 18 studies, data were estimated using data from different technologies, and only 1 study used MSMs, which is most likely due to the fact that MSMs have only recently been introduced for data estimation in LCA.

Several studies did not include any estimations of emissions and natural resource use. Emissions could probably be up-scaled from lab or pilot scale to commercial scale, but most lab-scale or pilot-scale studies did not report estimations of environmental emissions. The reason for that could be that the aim of these studies was to develop proof of concept at lab scale or to test a new process at pilot scale, and hence these studies did not focus on the estimation of emissions. Another reason could be that it is unclear how these emissions could be estimated because it is unclear what kind of chemical emissions could be formed during the process, as chemical species tend to react with each other, resulting in other chemical configurations. However, it is essential to estimate emissions in LCA of emerging technologies, and it is advisable to perform a review study on how the emission data could be estimated for future commercial-scale technologies, see e.g. Ma et al. (2019).

It should be noted that some methods have inherent constraints limiting their applicability to specific technologies; for example, stoichiometry (manual calculations) and MSMs can only be used for chemical technologies. However, MSMs are based on neural networks, and in theory, neural networks can be used for data estimation for technologies from different application domains. Neural networks have probably been used in data estimation in ex-post LCA, but only MSMs were found to be used in ex-ante LCA.

Based on our review findings, we summarized the key characteristics of data estimation methods used in ex-ante LCA in Table 3.3. As discussed before, we found that data estimation methods used in ex-ante LCA can be classified in the same classes as the data estimation methods applied in ex-post LCA (Parvatker and Eckelman 2019). It was noted that the data estimation methods used in ex-ante LCA had characteristics that were similar to those of the data estimation methods used in ex-post LCA described by Parvatker and Eckelman (2019).

***Table 3.3** Summary of key characteristics of data estimation methods used for up-scaling in ex-ante LCA.*

Up-scaling method	Results obtained	Tools and data needed	Expertise required	Advantages	Disadvantages	A[b]
Process simulation	Material/ energy inputs and outputs, elementary flows[a]	Simulation software, data on process operation conditions	1. Technology knowledge 2. Process design skills 3. Skills in software use 4. Engineering knowledge (e.g. chemical engineering in case of chemical technologies)	1. Calculations done by software are fast	1. Process design can be time consuming 2. Can be expensive (a license for software may be needed) 3. Requires detailed data on process conditions 4. Interpretation of simulation data might be challenging	1
Manual calculations	Material/ energy inputs and outputs, elementary flows	Equations, process operation conditions, yields of conversions, efficiency values	1. Technology knowledge 2. Engineering knowledge (e.g. chemical engineering in case of chemical technologies)	1. Inputs and outputs for most processes (e.g. stirring, filtration) can be calculated manually	1. Time consuming 2. Requires data on process conditions	2
Molecular Structure Models	Material inputs and outputs, elementary flows	Chemical structure of molecules	1. Basic knowledge in chemistry	1. Data estimation is fast and easy to perform 2. Data estimation is	1. It is applicable only to chemical technologies	3

				possible even if most of the data is lacking		
Use of proxy	Material/ energy inputs and outputs, elementa ry flows	Data for a proxy technology	1. Technology knowledge 2. Engineering knowledge	1. Data estimation is fast and easy to perform 2. Data estimation is possible even if most of the data is lacking	1. Data for a similar technology should be found	4

***Note:** the key characteristics of data estimation methods used in ex-ante LCA were similar to the characteristics given by Parvatker and Eckelman (2019) for the methods used in ex-post LCA.*

[a] Elementary flows = emissions and natural resource use; [b] A = Accuracy based on Parvatker and Eckelman (2019): the accuracy of the LCA results obtained after data estimation. 1 – the most accurate data estimation method and 4 – the least accurate data estimation method).

3.4.3 Decision tree

Based on the literature review results, we developed a decision tree that provides recommendations for up-scaling of an emerging technology in ex-ante LCA (Figure 3.3). In particular, the decision tree identifies the steps that should be taken when developing up-scaling scenarios including projected technology scenario definition, preparation of a projected flowchart, and the choice of a method for projected data estimation based on the availability of the data, the accuracy of the LCA results obtained after up-scaling (the methods listed at the top of the decision tree result in more accurate LCA results than the methods listed at the bottom), and the application domain. For data estimation, the same hierarchy in terms of data availability and accuracy can be used as for ex-post LCA (Parvatker and Eckelman 2019).

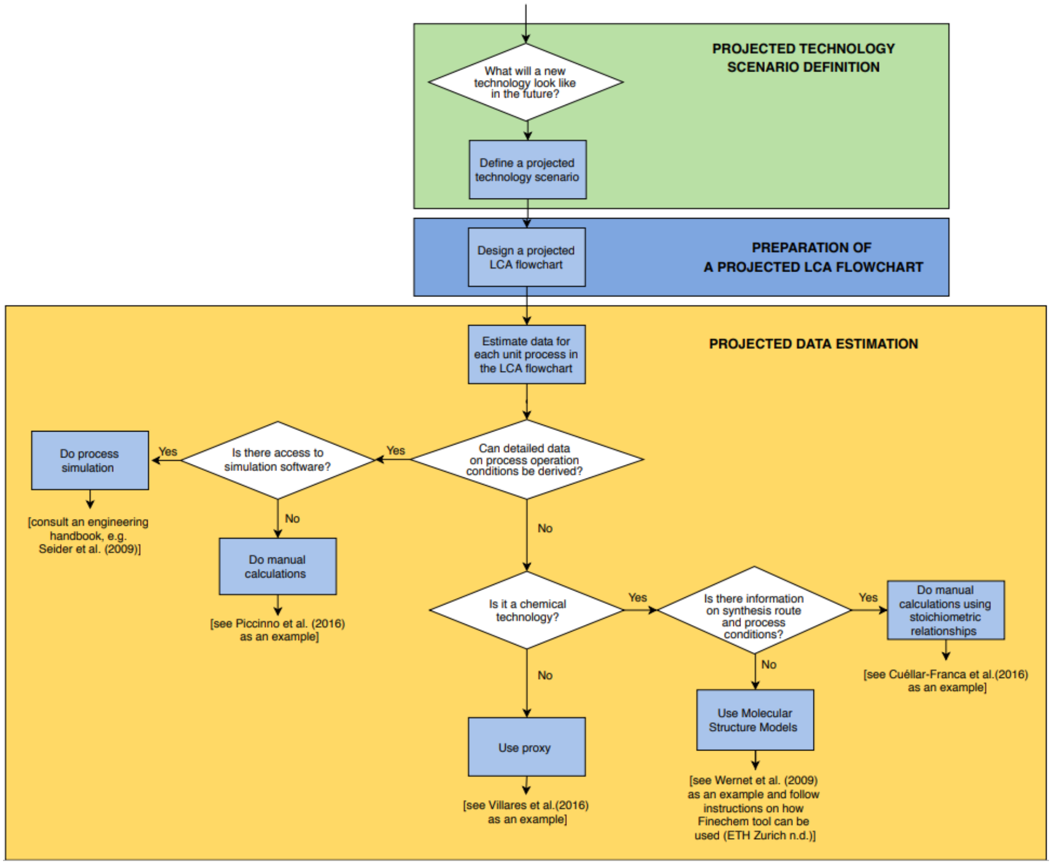

Figure 3.3 *Decision tree for up-scaling of an emerging technology in ex-ante LCA.*

The present review only captures up-scaling methods that have already been applied in ex-ante LCA. Methods that have not yet been applied or could not be applied in ex-ante LCA were not included in the review.

3.5 Conclusions and recommendations

This paper reviewed up-scaling methods applied in ex-ante LCA based on two sets of predefined criteria aiming to answer three questions:

1. Which up-scaling methods have already been applied in ex-ante LCA, and what are their key characteristics and methodological principles?
2. What steps are involved in the up-scaling of emerging technologies in ex-ante LCA?

3. Which recommendations can be given to practitioners of ex-ante LCA regarding up-scaling?

Regarding the first question, our findings show that most studies reported what a hypothetical up-scaled technology would look like in the future. In most studies, the authors did not describe in detail how the hypothetical up-scaled technology was designed. For instance, they did not report if technology experts were involved in the up-scaling. We recommend that up-scaling in ex-ante LCA is performed in cooperation by technology experts from different fields, such as technology developers, LCA experts, and engineers.

All studies described how they estimated data. In general, four data estimation methods were used: process simulation, manual calculations, MSMs, and using data from proxy technology. Remarkably, in most studies data was estimated using manual calculations, and only one study used MSMs. The use of MSMs for data estimation in LCA is currently being explored, which probably explains why MSMs have not been reported very often as being used in ex-ante LCA. Some studies estimated data using a mix of methods. It is unclear whether a mix of data estimation methods would lead to more accurate results than the use of only one method. Some methods have limitations in their applicability to specific technologies; for example, stoichiometry (manual calculations) and MSMs can only be used for chemical technologies.

None of the reviewed studies reported on the accuracy of the up-scaling results, i.e. the results of ex-ante LCA were not validated after the implementation of the new technology at industrial scale. We recommend validation of ex-ante LCA results once the technology is operating at full scale to check the accuracy of the up-scaling methods.

Furthermore, our findings show that studies up-scaled different kinds of technologies from different application domains, such as chemistry, waste treatment, energy, food, and the building sector. Most studies performed up-scaling for chemical and waste treatment technologies. All studies reported on how they estimated energy and material inputs and outputs, but not all of them reported on how they estimated emissions. Reporting on how emissions were estimated is important in LCA, and we recommend LCA practitioners to report on that. All studies described technologies by using the terms ‘lab-scale’, ‘pilot-scale’, ‘industrial-scale’ or ‘full-scale’, and some studies mentioned the expected production capacity of the up-scaled technology at pilot or industrial scale (Appendix C), but none of them specified TRLs. We recommend that LCA experts report on TRLs, since TRLs provide a much clearer indication of the maturity level of a technology than the general terms ‘lab-scale’, ‘pilot-scale’, ‘industrial-scale’ or ‘full-scale’ and production capacities.

Regarding the second question, we developed a framework based on our review results that can be used in the up-scaling of emerging technologies in ex-ante LCA. The framework consists of three main steps: 1) projected technology scenario definition, 2) preparation of a projected LCA flowchart and 3) projected data estimation. Each step involves different types of expertise, decisions, choices and assumptions. In the first step, a technology expert develops a scenario resembling a specific up-scaled emerging technology at pilot scale (TRL 6-8) or at industrial scale (TRL 9). The same technology expert may also specify required process operation conditions, installations, etc. for a technology at higher TRL. Then, in the second step, an LCA expert prepares LCA flowchart by using the results of the technology scenario definition step. In the third step, the LCA expert estimates data for each unit process defined in the LCA flowchart.

With regard to the third question, we conclude that there is no standard approach for up-scaling in ex-ante LCA. That is why there is no consensus among LCA practitioners on how up-scaling should be done. Thus, we developed a decision tree that recommends which steps should be followed in the up-scaling procedure and which methods should be used for data estimation based on the availability of the data, the accuracy of the results obtained after data estimation and the application domain. LCA practitioners can use this decision tree in their ex-ante LCA case studies, but they should also keep in mind that this decision tree gives a general overview of up-scaling procedures and that some alterations can be necessary for up-scaling in a particular case study.

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