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

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Summary

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The aim of this thesis was to explore the challenge of LCI modelling in prospective LCA. To be more specific, the thesis focused on methods used to upscale emerging chemical technologies and to model background scenarios for new technologies in prospective LCA.

In Chapter 2, we conducted LCA of new anti-reflective coating used in Dutch greenhouses. The primary challenge we identified was the need to upscale the production of the new coating. This challenge stemmed from the fact that the new coating was initially developed on a laboratory scale and had to be upscaled to match the production scale of conventional coatings. To tackle this challenge, we collaborated with technology developers to develop the pilot and industrial scale scenarios for the production of the new coating. A cradle-to-grave LCA was performed, and the functional unit was defined as the production of 1692.30 kg of tomatoes in greenhouses during 30 years.

The results of LCA showed that the newly developed coating, produced on an industrial scale, could compete with conventional coatings in terms of environmental performance. Additionally, the LCA indicated that while the evaluated new coating didn't offer significant environmental advantages compared to using uncoated glass, its application in greenhouses could yield economic benefits over its operational lifespan, particularly through enhanced crop yields (such as tomatoes). Various developmental trajectories of the novel coating technology were explored in the sensitivity analysis. Among these pathways, the option involving glass manufacturing in the Netherlands, as opposed to China, yielded the most favorable environmental impact outcomes.

Chapter 2 of this thesis highlighted the challenge of upscaling an emerging technology in LCA. Hence, chapter 3 addressed this challenge by conducting a comprehensive literature review of upscaling methods employed in ex-ante LCA. A total of 18 studies were selected for review, including a variety of technologies across diverse application domains including chemistry, waste treatment, energy, food, and the building sector. The review findings revealed that most studies developed scenarios on what a hypothetical upscaled technology would look like in the future. Furthermore, each study reported

data estimation using methods such as process simulation, manual calculations, molecular structure models (MSMs), and proxies.

Certain studies employed a combination of methods to estimate data. Some methods possess limitations regarding their suitability for particular technologies; for instance, stoichiometry (manual calculations) and MSMs are exclusively applicable to chemical technologies. While all studies reported their approaches for estimating energy and material inputs and outputs, not all of them provided information on estimating emissions. Reporting on the methodology used to estimate emissions in LCA is essential, and we strongly advise LCA practitioners to include this information in their studies.

As the review findings indicated a common pattern among ex-ante LCA studies in their upscaling approaches, we developed a framework for upscaling emerging technologies in ex-ante LCA. This framework comprises three primary steps: (1) projected technology scenario definition, (2) preparation of a projected LCA flowchart, and (3) projected data estimation. Additionally, based on the review findings, we developed a decision tree to offer guidance for LCA practitioners regarding the upscaling process in ex-ante LCA.

In Chapter 4 the upscaling framework developed in Chapter 3 was applied to an emerging Carbon Capture and Utilization (CCU) technology. This CCU innovation transforms CO and CO_2 from blast furnace gas (BFG) in a steel mill into polyols, which can subsequently be utilized in polyurethane production for coatings and rigid foam for insulation boards. The CCU technology spans a range of technology readiness levels (TRL) between TRL 2 and TRL 6, with various components such as gas conditioning and polyol production existing at different TRL levels within this range. Laboratory and pilot scale technology systems were upscaled to an anticipated industrial scale using the upscaling framework, providing an estimate of its prospective performance at full industrial capacity.

The LCA followed the ISO 14044 framework (ISO International Standard 14044 2006). The first step of the upscaling framework, namely "Projected technology scenario definition," was executed during the Scope definition phase of the LCA. Technology developers drafted three upscaled technology scenarios by designing Aspen Plus process flow sheets. The subsequent upscaling step, "Preparation of a projected LCA flowchart," was carried out within the Inventory analysis phase of the LCA. During this step, the Aspen Plus flowsheets were transformed into LCA flowcharts. The final step of the upscaling framework, "Projected data estimation," was also conducted in the Inventory analysis phase. Here, data for each unit process were estimated using two data estimation methods: technology developers utilized “process simulation” via Aspen Plus to calculate energy and material flows. Additionally, LCA experts employed another data estimation method, “manual calculations” (stoichiometric calculations). Subsequently, LCA computations were performed utilizing the outcomes of the upscaling steps as input. The environmental performance of three scenarios of the upscaled CCU system was compared to the incumbent steel and polyol systems (baseline system).

The LCA findings indicated that, while all three scenarios of the CCU technology demonstrated improved environmental performance compared to the incumbent technology, the improvement was constrained to a maximum reduction of approximately 10% in carbon footprint. Across all three scenarios, the primary hotspots in terms of life cycle impacts were found to be the energy and chemicals utilized in the production of CCU polyols.

In Chapter 5, we explored other challenges associated with the LCI modelling of chemical technology systems in prospective LCA in addition to the upscaling challenge discussed in Chapter 3. Firstly, reports and roadmaps were reviewed to determine which chemicals would play an important role in the future chemical industry and require focus in prospective LCA. Then a review of prospective LCA studies was carried out to identify which chemicals had been evaluated using prospective LCA and the approaches used to model prospective scenarios for future chemicals.

The review of reports and roadmaps revealed ammonia, methanol, hydrogen, and high-value chemicals as key future chemicals. Overall, 30 prospective LCA studies assessed these key chemicals and other chemicals such as polymer materials, nanomaterials, carbon allotropes, and fuels. These studies used various approaches to model future scenarios for chemical technologies. We categorized these approaches into three main groups such as 1) Existing scenario narratives/storylines, 2) Methods for generation of scenarios and 3) Scenario modelling methods and data sources. Each of these groups includes methods for generating and modelling scenarios, as well as scenario data sources. Certain methods and scenario data sources are suitable for foreground scenario modelling, others to background scenario modelling, and some for both. While reviewed studies predominantly concentrated on modelling foreground scenarios, they often neglected modelling prospective background scenarios. However, inclusion of prospective background scenarios accounting for expected future socio-economic developments is essential for evaluating potential environmental impacts of chemical technologies.

In Chapter 6, we addressed the research sub-questions initially outlined in the thesis introduction. By answering these sub-questions, we were able to address the main research question "How can we estimate the environmental impact throughout the life cycle of emerging chemical technology systems by exploring potential future scaled-up versions of the technology and projecting data for these upscaled versions?" As the response to this research question, we presented methods for upscaling emerging technologies, categorized them, and offered guidelines on the upscaling procedure, including the use of the upscaling framework and the decision tree. In addition, we provided an overview of methods for modelling prospective background scenarios, along with their classification.

Additionally, we provided insights into our work, including reflections and acknowledgments of its limitations. These limitations included, for example, the omission of modelling background scenarios for the CCU technology in the LCA case study after upscaling, as well as the recognition that the decision tree offers only a general overview of the procedure for selecting upscaling methods, potentially necessitating adjustments when applying it to upscale a specific new technology.

Lastly, we outlined potential topics for future research, aiming to advance LCI modelling and data estimation in prospective LCA. These include investigating methods for upscaling emissions for emerging chemical technologies, creating a framework for generating technology scenarios during the upscaling process of chemical technologies, and identifying sectors and chemicals that need to be included in prospective LCI background databases. Such improvements are highly policy relevant given the fact that many sustainability problems are to be solved by novel technologies, and that both policy as research programs need guidance on how to select the most promising future technologies.