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

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Chapter 5: Approaches to model future chemical production technologies in prospective Life Cycle Assessment

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Abstract

The chemical industry significantly contributes to carbon dioxide emissions, necessitating substantial reduction efforts. To address this challenge, the industry is actively developing greenhouse gas mitigation strategies. These include retrofitting facilities to utilize renewable feedstock and energy, implementing carbon capture technologies, and exploring other innovative solutions. Evaluating the environmental impact of future chemical production technology systems can be achieved through prospective Life Cycle Assessment (pLCA). Here, we first perform a review of reports and roadmaps that identifies which chemicals will play a key role in a future low carbon society and require focus in pLCA. We then review existing pLCA studies to identify which chemicals have been assessed using pLCA. Furthermore, we review pLCA studies to identify which approaches have been applied 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. The review identified 30 pLCA studies assessing these key chemicals and other chemicals such as polymer materials, nanomaterials, carbon allotropes, and fuels. Regarding the approaches that have been used to model prospective scenarios of chemicals, diverse approaches were observed across studies. We categorized these approaches into three groups 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 sources for scenario data. Some methods and scenario data sources are applicable to foreground scenario modelling, others to background scenario modelling, and some to both.

5.1 Introduction

The urgent need to address climate change is a matter of global concern. In 2015, the Paris Agreement was established with the objective of limiting the increase in global temperature to well below 2°C, with a preference for a maximum increase of 1.5°C above pre-industrial levels (United Nations, n.d.). To achieve this objective, global carbon dioxide (CO_2) emissions need to be reduced by 45% by 2030 relative to 2010 levels, while net-zero emissions should be realized by 2050 (United Nations, n.d.). Unfortunately, the world is currently not yet making sufficient progress towards meeting these targets (United Nations, n.d.), while 2023 was the year with the global average temperature being approximately 1.5°C above pre-industrial levels (The World Meteorological Organization, 2024). Thus, application of technologies for the climate change abatement is of high importance. Climate change mitigation technologies can be categorised into three groups (Fawzy et al., 2020):

1) Conventional mitigation technologies that aim at reducing fossil-based CO_2 emissions. Examples include renewable energy, nuclear power, fuel switch and efficiency gains, Carbon Capture and Storage (CCS) and Carbon Capture and Utilization (CCU).
2) Negative emissions technologies that are applied to capture and sequester carbon from the atmosphere. For example, bioenergy carbon capture and storage, biochar, afforestation and reforestation, ocean fertilization.
3) Geoengineering techniques of radiative forcing that focus on changing the earth's radiative energy budget to stabilize or lower global temperatures. For instance, stratospheric aerosol injection, space-based mirrors, and marine sky brightening.

Nowadays the chemical industry emits about 2 billion metric tons of CO_2 per year (direct and energy emissions), contributing to about 5% of global GHG emissions (Gabrielli et al., 2023). Thus, the chemical industry needs to make significant reductions in GHG emissions to meet the targets set by the Paris agreement.

To achieve these reductions, several chemical industry roadmaps and reports (Center for Global Commons and SYSTEMIQ, 2022; International Energy Agency, 2018; International Energy Agency et al., 2013; Material Economics, 2019; Shuyi et al., 2022; Stork et al., 2018) have been developed, suggesting various strategies that could help to mitigate GHG emissions by this sector. One example of these strategies is using group (1) of the climate change mitigation technologies mentioned above such as retrofitting current chemical facilities with supply-based emission mitigation solutions, e.g., transitioning from fossil to alternative feedstocks, switching from fossil to renewable energy sources, and implementing CCS (Center for Global Commons and SYSTEMIQ, 2022). Another strategy involves incorporating new chemical production technology systems, that are currently at a low technology readiness level (TRL), e.g., CCU technologies (Thonemann and Maga, 2020; Tsoy et al., 2023; Von Der Assen and Bardow, 2014).

While innovations may be claimed to be sustainable, it is essential to verify such claims by performing, for instance, early on environmental assessments. These assessments may help in making informed decisions about which innovations to support and invest in.

Life cycle assessment (LCA) has been widely used as a method for the environmental assessment of products and technology systems. Generally, LCA is applied to existing, mature technology systems (retrospective LCA (Arvidsson et al., 2023)). Innovative, emerging technology systems usually still have significant room for environmental and economic efficiency improvements when they scale up and penetrate larger markets. To capture such improvements, forward-looking LCA modes, e.g., anticipatory LCA, ex-ante LCA and prospective LCA (pLCA), have been developed in recent years, allowing to assess the environmental impacts of emerging technology systems (Cucurachi et al., 2018).

Although some LCA practitioners use the terms “ex-ante LCA” and “pLCA” interchangeably, others perceive differences between them. Van der Giesen et al. (2020a) state that “ex-ante LCA” refers to the assessment of a technology system before its market introduction, whereas “pLCA” refers to any forward-looking assessment that can thus also be carried out on an established technology system to identify its environmental impacts in the future. In this review, we will focus on LCA of chemical production technology systems that are currently at low TRL and are expected to be potentially implemented at the commercial scale. Also, we will review LCA of technology systems that have already been operating at the commercial scale (TRL 9) to assess their future environmental impacts. Thus, in this review paper, we will refer to the reviewed LCA studies as "pLCA" studies.

The execution of pLCA poses various challenges. First, foreground processes for which data are available at low TRLs need to be upscaled to a situation where the technology system is mature and has penetrated the market. Second, background processes have to be modelled to represent a future situation. Third, these two challenges imply that uncertainties in the pLCA may become even more pronounced as in regular LCAs. Various studies have discussed these challenges and proposed potential solutions to them (Buyle et al., 2019; Moni et al., 2020; Thonemann et al., 2020; Tsoy et al., 2020; van der Giesen et al., 2020b). In this study, our objectives are to determine chemicals that will play a key role in the future chemical industry and to identify methods that could be used to estimate pLCA data of the production of these chemicals. The term "pLCA data" refers to inventory data for future projections of chemical production processes.

Thus, we aim to answer the following research question and related sub-questions:

Which approaches are available to model future foreground and background scenarios for key chemicals in pLCA?

1. What are the key chemicals that are expected to play an important role in the future, and what are their potential future production routes? (Section 5.2)
2. Which of the key chemicals identified have been assessed using pLCA? Additionally, for which other chemicals have pLCAs been conducted? (Section 5.3.2.1)
3. What can be learned from existing pLCA studies of the key chemicals? Additionally, which methods are available from pLCAs of other chemicals that could be applied to model key chemicals? (Section 5.3.2.2)

Section 5.2 will address sub-question "What are the key chemicals that are expected to play an important role in the future, and what are their potential future production routes?" by reviewing reports and roadmaps on the future structure of the chemical industry, which will be highly influenced by climate change mitigation ambitions. The outcomes of this review will help to determine which chemicals and innovative production processes are expected to become important and for which pLCA hence are relevant. In section 5.3, the sub-questions 2 and 3 will be addressed by conducting a review of pLCA studies. This section will discuss the chemicals/chemical products assessed in pLCA studies. Also, the review results will help to determine prospective scenario modelling approaches that could be used to model key chemicals. Sections 5.2 and 5.3 will be followed by a Discussion and Conclusion section.

5.2 Key chemicals, their production volumes and production routes

5.2.1 Methods

For answering sub-question 1, we reviewed reports and roadmaps that discussed the future structure of the chemical industry, particularly in view of climate change mitigation targets. The Industry Transition Tracker (Johnson et al., 2020) database was used to search for such reports. The database offers a platform for searching reports based on different criteria such as countries, actors, sectors, and roadmap enablers. In this study, "Chemicals" was selected as the "sector in focus" to search for reports. Out of 38 reports found, 14 were selected for further review, while 24 were excluded as:

- 16 reports had a status of pending validation.
- 5 reports were published in other languages than English.
- 3 reports were not available online.

In addition to 14 reports found via the Industry Transition Tracker, 5 reports were added to the review by snowballing. Thus, in total, 19 reports were included in this study (Table E1 in Appendix E).

5.2.2 Results

5.2.2.1 Identification of key chemicals of the future chemical industry

Several reports discussed future developments of the industry sector in general, but covered next to the cement, steel and other industrial sub-sectors the chemical industry as well. Other reports focused on chemical industry specifically. Approximately half of reports (Bazzanella and Ausfelder, 2017;

Center for Global Commons and SYSTEMIQ, 2022; International Energy Agency, 2021a, 2012; International Energy Agency et al., 2013; Material Economics, 2019, 2018; Shuyi et al., 2022; Stork et al., 2018; Sustainable Development Solutions Network and Fondazione Eni Enrico Mattei, 2021) indicated that they had a specific focus on chemicals (Table E1 in Appendix E). Given climate mitigation targets, several reports highlighted key chemicals relevant for a low-carbon chemical industry such as ammonia (Bazzanella and Ausfelder, 2017; Center for Global Commons and SYSTEMIQ, 2022; International Energy Agency, 2021a; International Energy Agency et al., 2013; Material Economics, 2019; Shuyi et al., 2022; Stork et al., 2018), methanol (Bazzanella and Ausfelder, 2017; Center for Global Commons and SYSTEMIQ, 2022; International Energy Agency et al., 2013; Shuyi et al., 2022; Stork et al., 2018), and high-value chemicals (Bazzanella and Ausfelder, 2017; Center for Global Commons and SYSTEMIQ, 2022; International Energy Agency et al., 2013; Shuyi et al., 2022; Stork et al., 2018). Hydrogen was reported in most reports both as a separate chemical and as a feedstock for other chemicals such as ammonia, methanol, etc. Other chemicals that were reported less frequently as the main focus of the reports were biofuels, plastics, synthetic fuels, chlorine. The remaining reports (British trade association representative jointly led by British government and industry, 2015; Cefic, 2019; Entreprises pour l'environnement, 2019; International Energy Agency, 2019; Ministry for the Ecological and Solidary Transition (France), 2020; Montalvo et al., 2019; SEMARNAT and INECC, 2016; The négaWatt Association, 2017; WBCSD, 2018) did not have a specific focus on any particular chemicals.

In this paper we decided to focus on future production routes of key chemicals: ammonia, methanol and high-value chemicals. The term "high-value chemicals" refers to light olefins (ethylene, propylene) and BTX aromatics (benzene, toluene, mixed xylenes). The selection of these chemicals was made due to the fact that the reviewed reports identified these chemicals as the focus of their work more frequently. These reports explored potential future developments for these chemicals, e.g., possible decarbonization pathways. Consequently, it can be concluded that these chemicals will play an important role in the future chemical industry, considering the emphasis placed on them as the focus in the reviewed reports. We further included hydrogen in addition to these key chemical groups. We did so since hydrogen is expected to play a key role in low-carbon ammonia and methanol production.

It is worth to mention that the chemical industry produces thousands of chemicals, most of them are derived from the key chemicals such as ammonia, methanol and high-value chemicals (International Energy Agency, 2018; Meng et al., 2023). Currently, these chemicals account for nearly two-thirds of the total energy consumed by the chemical sector (International Energy Agency, 2018). Figure 5.1 shows the basic role these key chemicals play in the chemical industry, and the pathways through which more complex chemicals and end use products can be produced from them.

5.2.2.2 Future production volumes and production routes of key chemicals

The previously discussed reports did not present future scenarios regarding the volumes and production technology shares of the key chemicals, with the exception of Center for Global Commons and SYSTEMIQ (2022). Consequently, in this section, apart from the Center for Global Commons and SYSTEMIQ (2022) contribution, we incorporated reports International Energy Agency (2021b), IRENA and AEA (2022), and International Energy Agency (2018) to explore future developments of key chemicals. It is important to highlight that these reports covered scenarios specifically related to certain key chemicals and did not address all key chemicals. Therefore, the depiction of scenarios for one key chemical may differ from those for another key chemical within this section.

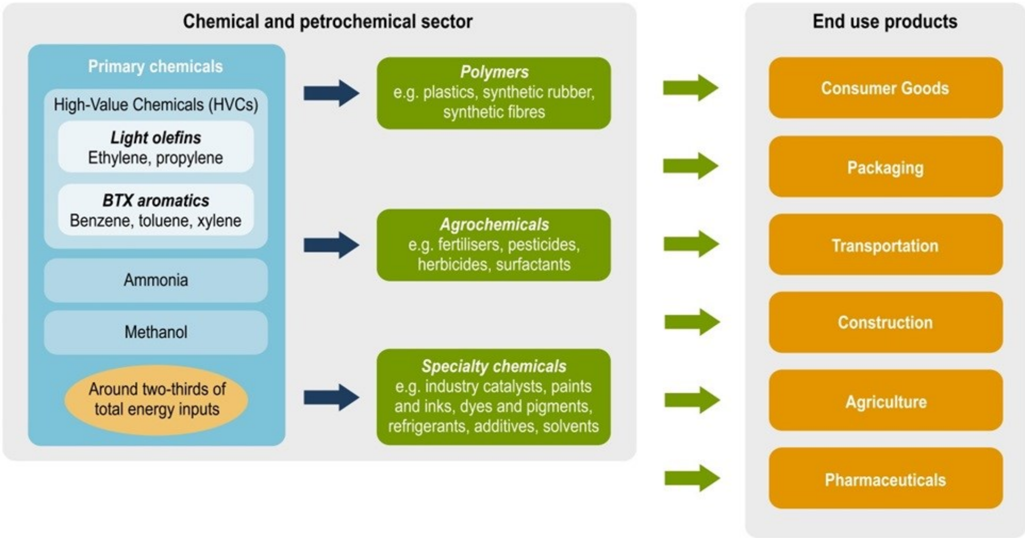

***Figure 5.1** Key chemicals and their use (Source:* International Energy Agency (2018)*).*

Ammonia

Ammonia is one of the large-scale produced chemicals worldwide. In 2020, the global ammonia production equalled to 185 million tons per year (Mt/year), accounting for 27% of the total chemicals production (Meng et al., 2023). Nearly 70% of ammonia is used for making mineral nitrogen fertilizers for food production (International Energy Agency, 2021b). Furthermore, ammonia is used as a chemical building block to produce various industrial products such as cleaning products, explosives (International Energy Agency, 2018) and pharmaceuticals (Bazzanella and Ausfelder, 2017). Currently ammonia (NH_3) is mainly produced via the Haber-Bosch process, in which atmospheric nitrogen (N_2) reacts with hydrogen (H_2) using a catalyst (Smith et al., 2020). Nitrogen for the Haber-Bosch process is obtained from the atmosphere, while hydrogen is generated via different routes: about 54% comes from gas-based production, 21% from coal-based production, 1% from oil-based production, 23% from fossil-based production coupled with CCU, and a fraction of a percentage point from gas-based production with CCS and electrolysis (International Energy Agency, 2021b).

Different scenarios project increased production of ammonia in 2050. Figure 5.2 shows expected volumes for ammonia production in the IEA and IRENA scenarios in 2050. The IEA Stated Policies Scenario reflects the ammonia sector's current trajectory, influenced by existing and announced policies (International Energy Agency, 2021b). The IEA Stated Policies Scenario indicates a trajectory that would lead to a 2.5 °C temperature rise in 2100 (International Energy Agency, 2022). According to the IEA Stated Policies Scenario, ammonia production for the chemical and agricultural sectors is expected to increase from current levels to 253 Mt/yr in 2050, driven primarily by economic and population growth (International Energy Agency, 2021b). In the IEA Sustainable Development Scenario, the sector adopts the technologies and policies required to put it on a pathway aligned with the goals of the Paris Agreement, and this will lead to slightly lower ammonia production levels reaching approximately 228 Mt/yr compared to the IEA Stated Policies Scenario (International Energy Agency, 2021b). The IEA Net Zero Emissions by 2050 Scenario is more ambitious than the IEA Sustainable Development Scenario. The IEA Net Zero Emissions by 2050 Scenario describes a trajectory for the ammonia industry compatible with reaching net zero emissions globally for the energy system by 2050 (International Energy Agency, 2021b). In the IEA Net Zero Emissions by 2050 Scenario, the global temperature rise peaks below 1.6 °C around 2040, before dropping to around 1.4 °C in 2100 (International Energy Agency, 2022). In this scenario, ammonia production will reach 227 Mt/yr which is approximately the same as in the IEA Sustainable Development Scenario (International Energy Agency, 2021b).

The IRENA scenarios consider new possible applications such as its use as a hydrogen carrier, fuel for shipping and power generation (in addition to ammonia's conventional applications for the chemical and agricultural sectors). According to the IRENA 1.5°C scenario (IRENA and AEA, 2022), the total ammonia production including conventional and new applications will account for 688 Mt/yr. To be more specific, under this scenario, ammonia demand for its conventional uses is projected to increase to 334 Mt/year from today, with 267 Mt/year for fertilizer applications and 67 Mt/year for other existing markets. With regards to new applications of ammonia, the IRENA 1.5°C scenario (IRENA and AEA, 2022) expects that ammonia demand for its use as a hydrogen carrier, fuel for shipping, and power generation will rise from zero today to 354 Mt/year by 2050. Specifically, 127 Mt/year of ammonia will be produced for use as a hydrogen carrier, 197 Mt/year of ammonia will be used as a maritime fuel, and 30 Mt/year of ammonia will be used for power generation. Less ambitious scenario, IRENA Stated Policies Scenario, projects lower ammonia production numbers compared to IRENA 1.5°C scenario. In the IRENA Stated Policies Scenario (IRENA and AEA, 2022), total ammonia demand, including the conventional uses and new applications, will reach 550 Mt/yr in 2050. The difference in ammonia volumes in these scenarios is mainly due to the fact that IRENA Stated Policies Scenario sees lower share of ammonia's demand as a hydrogen carrier and as a fuel for shipping than those in IRENA 1.5°C scenario. In IRENA Stated Policies Scenario, ammonia's demand as a hydrogen carrier and as a fuel for shipping are expected to be 109 Mt/yr and 77 Mt/yr, respectively.

IRENA and AEA (2022) expect that the Haber-Bosch process will remain the main technology for ammonia production at industrial scale in the future. Technically, low-CO_2 emission production of ammonia is possible using the same Haber-Bosch process as is used nowadays, but the crux is the inputs to this process: electricity and hydrogen (Material Economics, 2019). A greater share of renewable electricity and green/blue hydrogen in the Haber-Bosch process could lead to decreased indirect CO_2 emissions (Center for Global Commons and SYSTEMIQ, 2022).

In the IEA ammonia technology roadmap (International Energy Agency, 2021b), IEA presented shares of the technologies for the global production of hydrogen for Haber-Bosch in 2020 and the IEA scenarios in 2050 (figure 5.3).

The IEA Stated Policies Scenario (International Energy Agency, 2021b) expects for 2050 the following shares of technologies for production of hydrogen for the Haber-Bosch process: about 55% for gas-based production, 11% for coal-based production, 32% for fossil-based production coupled with CCU, approximately 1% for oil-based production, and less than 1% for electrolysis and gas-based production with CCS. The IEA Sustainable Development Scenario (International Energy Agency, 2021b) expects a lower share of gas-based production (about 22% of ammonia production), coal-based production (4% of ammonia production), and fossil-based production with CCU (24% of ammonia production) compared to the IEA Stated Policies Scenario. This IEA Sustainable

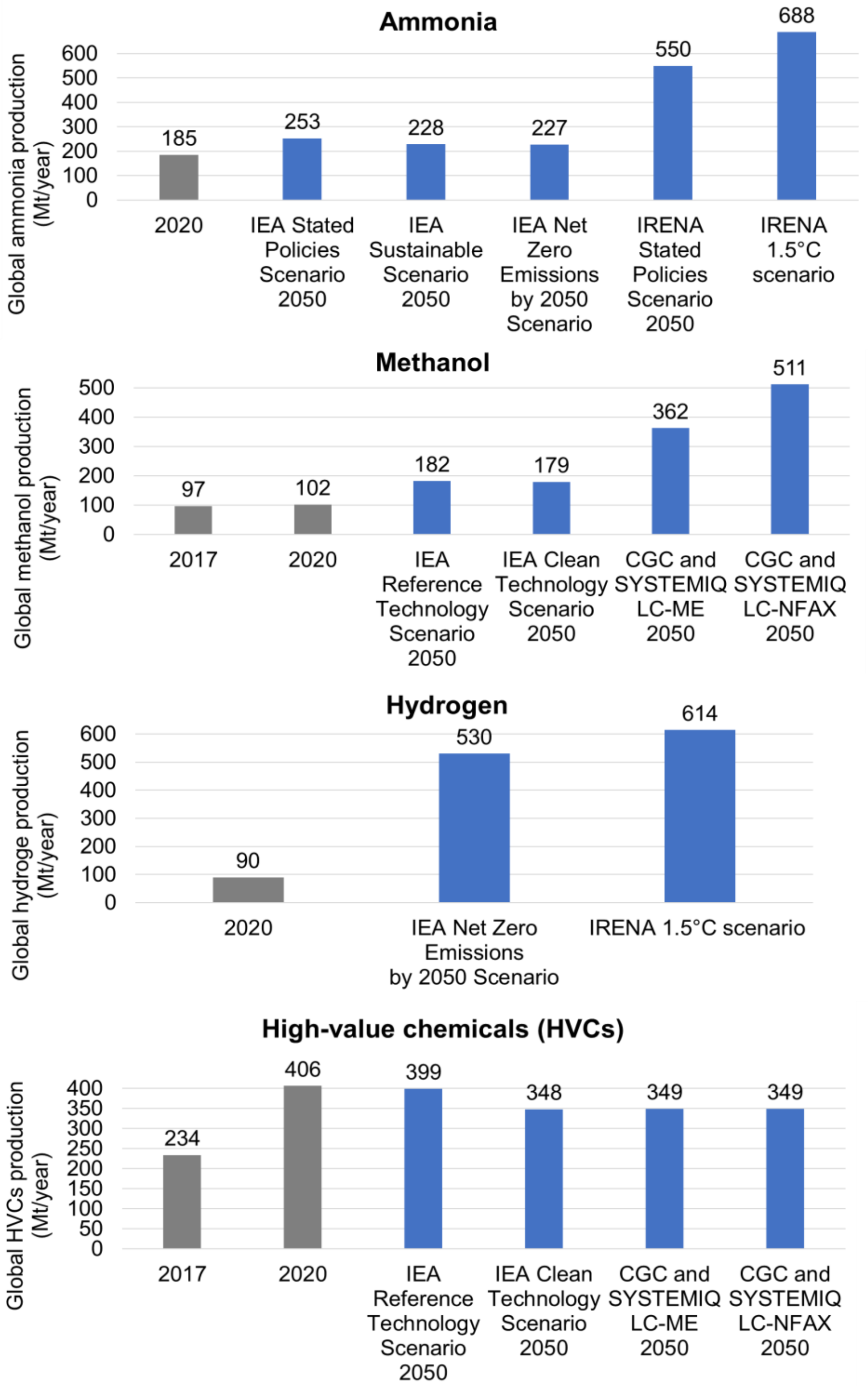

Figure 5.2 *Global production of ammonia, methanol, hydrogen and high-value chemicals in 2017 and/or 2020 and 2050. The charts were prepared*

*based on the data from International Energy Agency (2021b) and IRENA and AEA (2022) (for ammonia); International Energy Agency (2018) and Center for Global Commons and SYSTEMIQ (2022) (for methanol); International Energy Agency (2021c) and International Renewable Energy Agency (2022) (for hydrogen); International Energy Agency (2018) and Center for Global Commons and SYSTEMIQ (2022) (for high-value chemicals). *The IEA scenarios for ammonia production do not include new possible future applications of ammonia such as its use as a hydrogen carrier, fuel for shipping and power generation, while IRENA scenarios include future new applications.*

Development Scenario projects higher share of gas-based production with CCS (about 20% of ammonia production) and electrolysis (about 27% of ammonia production). Furthermore, the IEA Sustainable Development Scenario expects that methane pyrolysis may show up as emerging technology producing hydrogen for ammonia production, constituting a small share of about 3%. The more ambitious IEA Net Zero Emissions by 2050 Scenario (International Energy Agency, 2021b) expects an even higher share of gas-based production with CCS (22% of ammonia production) and electrolysis (41% of ammonia production) compared to the IEA Sustainable Development Scenario. Moreover, in the IEA Net Zero Emissions by 2050 Scenario, emerging technologies such as methane pyrolysis and biomass gasification are expected to operate in 2050, accounting to 7% and 3% of ammonia production, respectively. The remaining 27% is provided by coal-based production (with and without CCS), gas-based production without CCS, and fossil-based production with CCU.

A great variety of new technologies for ammonia production has been researched, e.g. electrified steam methane reforming, electrochemical production, biological enzymes, chemical looping and low-temperature catalytic synthesis (Cherkasov et al., 2015; International Energy Agency, 2021b; Smith et al., 2020). Currently, these technologies are at TRL 4 or lower, and would need considerable development to reach commercial scale (TRL 9) (International Energy Agency, 2021b; IRENA and AEA, 2022). Thus, the IEA ammonia technology roadmap did not consider these technologies in the IEA scenarios (International Energy Agency, 2021b). However, uncertainties are associated with the development of innovations, and the advances may occur faster than expected, so that the new technologies (mentioned above) may play a role in the sustainable production of ammonia in the future (International Energy Agency, 2021b).

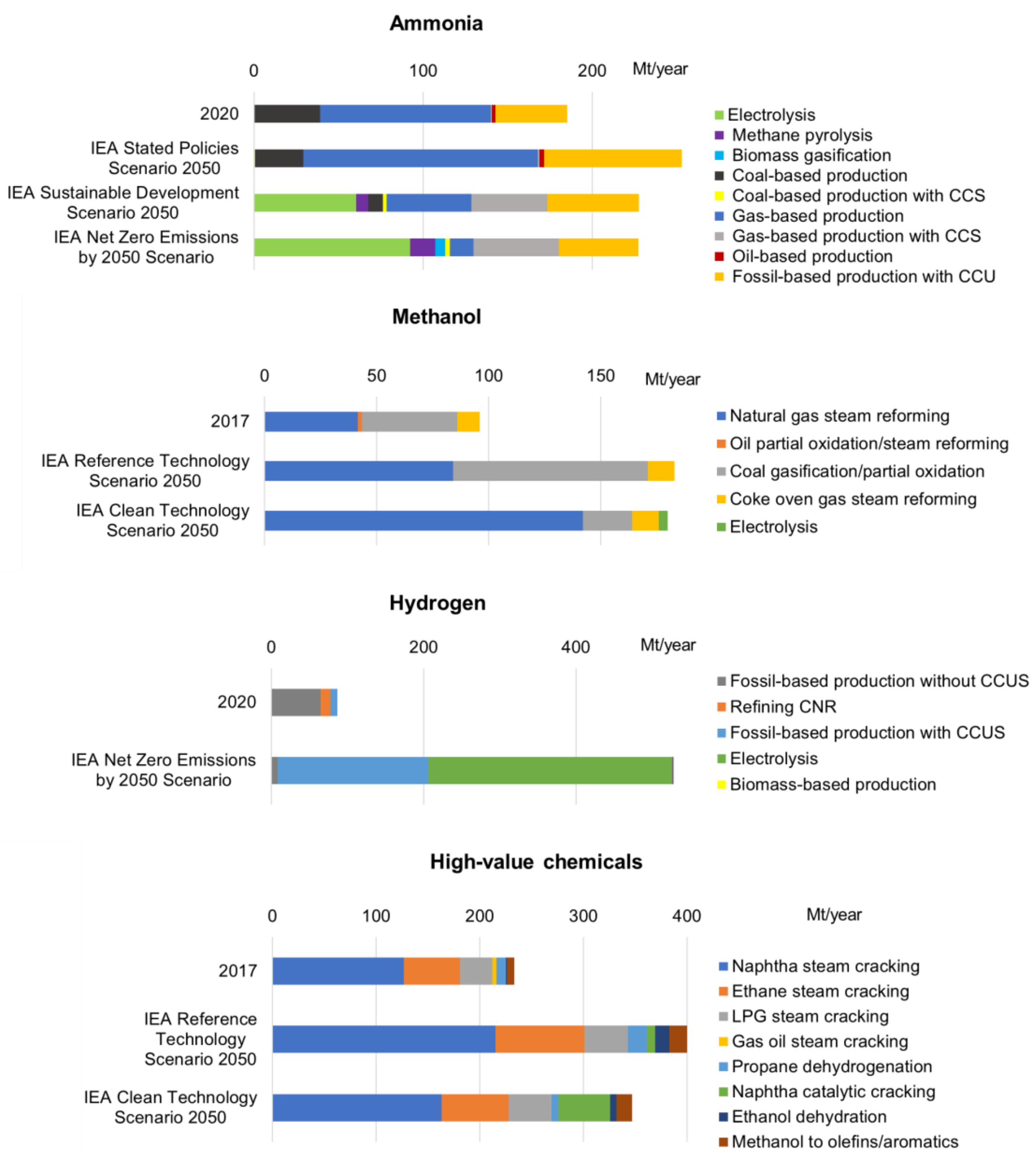

***Figure 5.3** Shares of production routes for ammonia, methanol, hydrogen and high-value chemicals in 2017 and/or 2020 and 2050. The chart was prepared*

based on the data from International Energy Agency (2021b) (for ammonia); International Energy Agency (2018) (for methanol); International Energy Agency (2021d) (for hydrogen); International Energy Agency (2018) (for high-value
*chemicals).*Refining CNR = hydrogen byproduct from catalytic naphtha ref orming at refineries; LPG = liquefied petroleum gas; *The IEA scenarios for ammonia production do not include new possible future applications of ammonia such as its use as a hydrogen carrier, fuel for shipping and power generation.*

Methanol

Methanol - the simplest alcohol – is commonly used as a building block to produce other chemicals (International Energy Agency, 2018; Meng et al., 2023). The global methanol production accounted for about 97 Mt/year in 2017 and increased to 102 Mt/year in 2020 (International Energy Agency, 2018; Meng et al., 2023). Around 40% of produced methanol is transformed into formaldehyde, and then used in the manufacture of variety of products, e.g., plastics, paints, textiles, plywood and explosives (International Energy Agency, 2018). Also, it can be utilized in solvents, transportation fuel, anti-freeze or serve as an energy carrier (International Energy Agency et al., 2013). In 2017, the global production of methanol was based mainly on coal gasification and partial oxidation (44% of methanol production), natural gas steam reforming (43% of methanol production), and coke oven gas steam reforming (10% of methanol production) (Figure 5.3).

Several scenarios project higher global methanol production in 2050 than in 2017 (Figure 5.2). The IEA Reference Technology Scenario (International Energy Agency, 2018) expects the production to increase to 182 Mt/year. This increase is mainly due to two relatively new methanol applications: its use as a fuel additive and as a building block for high-value chemicals production (International Energy Agency, 2018). The IEA Clean Technology Scenario (International Energy Agency, 2018) expects production to increase from today's levels to 179 Mt/year. According to the Center for Global Commons and SYSTEMIQ (2022) scenarios, the methanol production is expected to vary between 362 Mt/year and 511 Mt/year by 2050. These numbers are based on an expected significant increase in demand for methanol for high-value chemicals production (via the "Methanol to olefins/aromatics" route) from 31 Mt/year in 2020 to 290-439 Mt/year in 2050, while demand for methanol for other chemical production will be 72 Mt/year in 2050, the same as in 2020.

International Energy Agency (2018) reported shares of the global methanol production by technology in 2017 and in the IEA scenarios in 2050 (Figure 5.3). In the IEA Reference Technology Scenario (International Energy Agency, 2018), methanol will be produced mainly via coal gasification, partial oxidation and natural gas steam reforming, constituting to 48% and 46%, respectively, of total methanol production. Coke oven gas steam reforming will account for a small share, which will be about 7%. In the Clean Technology Scenario (International Energy Agency, 2018), shift from coal-based production to natural gas-based production is expected to occur. As a result, natural gas-based production will account for 79%, while coal-based production will be only 12%. Furthermore, methanol production using hydrogen produced via electrolysis will be used accounting to about 2%.

Hydrogen

Global demand of hydrogen was about 90 Mt/year in 2020 (International Energy Agency, 2021d). About 75% of hydrogen is produced via fossil-based production route, 15% of hydrogen is produced as a by-product in the catalytic naphtha reforming process, and the remaining hydrogen is produced via fossil-based production route with CCUS (Figure 5.3) (International Energy Agency, 2021d). Nearly 43% of hydrogen is used as feedstock, reagends, or energy source in refineries, about 37% of hydrogen is used for ammonia production, 15% of hydrogen for methanol production, the remaining share of hydrogen was used for the direct reduced iron process for steelmaking (International Energy Agency, 2023a, 2021c).

The IEA and IRENA scenarios expect that the global hydrogen demand will raise in 2050 (Figure 5.2). The IEA Net Zero Emissions by 2050 Scenario (International Energy Agency, 2021c) expects that hydrogen demand will increase almost sixfold from the demand volume in 2020 to 530 Mt/year in 2050. Such increase is explained due to the rising demand of hydrogen for heavy industry, road transport and shipping (International Energy Agency, 2021d). IRENA 1.5°C (International Renewable Energy

Agency, 2022) expects even higher global hydrogen demand of 614 Mt/year in 2050.

The IEA Net Zero Emissions by 2050 Scenario (International Energy Agency, 2021d) expects that electrolysis-based hydrogen will constitute about 60% of global hydrogen produced. About 38% of hydrogen will be produced via fossil-based production route with CCUS, approximately 2% of hydrogen will be generated via fossil-based production route without CCUS, and biomass-based production will account for only 0.2% (Figure 5.3) (International Energy Agency, 2021d).

High-value chemicals

In 2017, high-value chemicals production was 234 Mt/year (International Energy Agency, 2018), while in 2020 this number increased to 406 Mt/year (Center for Global Commons and SYSTEMIQ, 2022). The olefins are used in a great variety of products, mostly polymers (84%) (Meng et al., 2023). Light olefins (ethylene, propylene and butadiene), accounted for 290 Mt/year in 2020 (Center for Global Commons and SYSTEMIQ, 2022). BTX aromatics are the key chemical building blocks for consumer products such as pharmaceuticals (e.g., aspirin), textiles, packaging and refrigerants (Meng et al., 2023; The Aromatics Producers Association, n.d.). The global demand of BTX aromatics was 116 Mt/year in 2020 (Center for Global Commons and SYSTEMIQ, 2022).

Different scenarios expect decreased high-value chemicals production in 2050. The IEA Reference Technology Scenario expects that high-value chemicals production will reach 399 Mt/year, while the IEA Clean Technology Scenario expects demand to be 348 Mt/year. The Center for Global Commons and SYSTEMIQ (2022) scenarios project approximately the same production volume as the IEA Clean Technology Scenario (Figure 5.2).

The IEA Reference technology scenario expects that naphtha steam cracking, ethane steam cracking and liquefied petroleum gas (LPG) steam cracking will constitute the majority of the high-value chemicals production in 2050, contributing to 54%, 22% and 11% of total high-value chemicals production, respectively. Other technologies such as propane dehydrogenation, naphtha catalytic cracking, ethanol dehydration and methanol to olefins/aromatics will account for a smaller share (5%, 2%, 4% and 4%, respectively). In the IEA Clean Technology Scenario (International Energy Agency, 2018), decreased shares of naphtha steam cracking (47%), ethane steam cracking (19%) are expected. The share for LPG steam cracking will slightly increase to 12%. Naphtha catalytic cracking is expected to increase to 14%. Methanol to olefins/aromatics is expected to remain to be the same (4%). Ethanol dehydration and propane dehydrogenation will account for about 2% each (Figure 5.3).

5.3 Review of approaches to model prospective Life Cycle Inventories of chemicals

5.3.1 Methods

We conducted a literature search using the Web of Science database for 1990 to June 2023 for answering the sub-questions:

- Which of the key chemicals identified have been assessed using pLCA? Additionally, for which other chemicals have pLCAs been conducted?
- What can be learned from existing pLCA studies of the key chemicals? Additionally, which methods are available from pLCAs of other chemicals that could be applied to model key chemicals?

The following keywords were used in the search: "anticipatory Life Cycle Assessment" (Topic) OR "anticipatory Life Cycle Analysis" (Topic) OR "anticipatory LCA" (Topic) OR "prospective Life Cycle Assessment" (Topic) OR "prospective Life Cycle Analysis" (Topic) OR "prospective LCA" (Topic) OR "ex-ante Life Cycle Assessment" (Topic) OR "ex-ante Life Cycle Analysis" (Topic) OR "ex-ante LCA" (Topic). These keywords were searched in the titles and the abstracts of the studies. The studies found through the Web of Science database were then screened based on their titles and abstracts, and those that met the following exclusion criteria were not considered:

- Studies that did not carry out an LCA for an emerging chemical technology system (TRL<9) or future developments of a mature chemical technology system (TRL=9).
- Retrospective LCA studies.

- Studies that carried out an LCA of an emerging technology system at the laboratory/pilot scale but did not upscale them.
- Studies for which it was unclear whether an emerging technology system was upscaled or not and/or how it was upscaled (e.g., it was unclear at which scale (lab, pilot)/TRL an innovation was developed or to what scale (pilot, industrial)/TRL it was upscaled).
- Studies that did not clearly describe how they created scenarios or estimated prospective foreground/background LCA data.
- Studies that modelled renewable energy inputs to incumbent technology but did not report on the future time coverage, e.g. years.

Studies that did not meet the exclusion criteria were further reviewed.

5.3.2 Results

A total of 210 studies were identified using the Web of Science database. Following screening based on exclusion criteria, 26 pLCA studies were selected. Additionally, 4 pLCA studies were found via snowballing and included for review. Thus, in total 30 studies were reviewed (Table E2 in Appendix E). This section presents the findings of the literature review, organized into two sub-sections. The first sub-section provides a description of the chemicals assessed in the reviewed pLCA studies, while the second sub-section outlines the methods used to estimate pLCA data applied in these studies.

5.3.2.1 General description of chemicals/chemical products assessed in pLCA studies

The studies (Boyce et al., 2024; Delikonstantis et al., 2021; Delpierre et al., 2021; Lamers et al., 2023; Puig-Samper et al., 2022; Rosental et al., 2020; Thonemann and Maga, 2020; Valente et al., 2020; Wei et al., 2024) assessed the key chemicals as defined in section 5.2. Table 5.1 includes a list of future possible production routes for these key chemicals based on the IEA scenarios (described in Section 5.2) and a list of pLCA studies that carried out pLCA for each production route.

Table 5.1 *Key chemicals assessed in the pLCA studies.*

Key chemicals	Possible future production processes in 2050 (based on International Energy Agency (2021b) and International Energy Agency (2018))	Studies that assessed production of key chemicals
Ammonia production	Haber-Bosch process using hydrogen generated via processes (that can be equipped with CCS):	
	Electrolysis	Boyce et al. (2024)
	Gas-based production	Boyce et al. (2024)
	Coal-based production	Boyce et al. (2024)
	Oil-based production	Boyce et al. (2024)
	Biomass gasification	–
	Fossil-based production with CCU	Boyce et al. (2024)
	Methane pyrolysis	Boyce et al. (2024)
Methanol production	Production processes (that can be equipped with CCS):	
	Electrolysis for hydrogen production	Rosental et al. (2020); Thonemann and Maga (2020)
	Natural gas steam reforming	–
	Coal gasification/partial oxidation	–
	COG steam reforming	–
Hydrogen production	Production processes (that can be equipped with CCS):	
	Fossil-based production with CCUS	Wei et al. (2024)
	Biomass-based production	Valente et al. (2020); Wei et al. (2024)
	Fossil-based production	Valente et al. (2020); Wei et al. (2024)
	Electrolysis	Delpierre et al. (2021);

		Lamers et al. (2023); Puig-Samper et al. (2022); Valente et al. (2020); Wei et al. (2024)
High-value chemicals production	Production processes (that can be equipped with CCS):	
	Naphtha steam cracking	–
	Ethane steam cracking	–
	LPG steam cracking	–
	Propane dehydrogenation	–
	Naphtha catalytic cracking	–
	Ethanol dehydration	–
	Methanol to olefins/aromatics (using nonrenewable/renewable methanol)	Rosental et al. (2020)

The reviewed studies conducted pLCAs of hydrogen produced generated through electrolysis (Delpierre et al., 2021; Lamers et al., 2023; Puig-Samper et al., 2022; Valente et al., 2020; Wei et al., 2024), fossil-based production (with and without CCS) (Valente et al., 2020; Wei et al., 2024), fossil-based production with CCUS (Wei et al., 2024), and biomass gasification (Valente et al., 2020; Wei et al., 2024). In case of methanol, the studies assessed methanol production via CCU using hydrogen generated through electrolysis (Rosental et al., 2020; Thonemann and Maga, 2020) and plasma-assisted dry methane reforming-based process (Delikonstantis et al., 2021). With regards to ammonia, Boyce et al. (2024) modelled different kinds of technologies of ammonia production. Only one route for high-value chemicals production was assessed: Rosental et al. (2020) conducted a pLCA of the "Methanol to olefins/aromatics" route (Table 5.1, Table E2 in Appendix E).

Besides the key chemicals discussed in Section 5.2, we also reviewed literature applying pLCA to other chemicals/chemical products (Table E2 in Appendix E). We identified pLCA studies for a range of polymer materials, including bio-based carbon-fiber-reinforced polymers composites (Abbate et al., 2022), polyhydroxyalkanoates (del Oso et al., 2023a), biocomposite film (Günkaya and Banar, 2016), inorganic polymer (Joyce et al., 2018), biopolymer film (Müller-Carneiro et al., 2023), proteins (Röder et al., 2022), and starch (da Silva et al., 2021). Almost all these materials are produced using biomass as input material, with the exception of inorganic polymer produced using bauxite residue (Joyce et al., 2018).

Other studies assessed nanomaterials such as cellulose nanosponges (Bartolozzi et al., 2020), fibers covered with silver nanoparticles (Manda et al., 2015), acetylated cellulose nanofiber-reinforced polylactic acid (Kanematsu et al., 2021), and vanadium dioxide film (Sirvent et al., 2022) (Table E2 in Appendix E).

Carbon allotropes such as graphene (Arvidsson and Molander, 2017; Cossutta et al., 2017) and graphite (Kulkarni et al., 2022) were also assessed using pLCA (Table E2 in Appendix E). The assessment of graphene production routes encompassed epitaxial graphene growth, electrochemical exfoliation of graphite, chemical oxidation of graphite with chemical or thermal reduction, and chemical vapor deposition. The production route for graphite involved electrochemical graphitization.

Other studies assessed fuels, including hydrocarbon fuels for aviation (Ballal et al., 2023), REDIFUEL (fuel that consists of a mixture of high-cetane hydrocarbons and C_6-C_{11} alcohols) for road transport (van den Oever et al., 2023), drop-in biofuels (Watanabe et al., 2022) for shipping. Almost all fuels were produced from biomass. On the other hand, the hydrocarbon fuels were produced by combining H_2 and CO (obtained from captured CO_2) via the Fischer-Tropsch process (Table E2 in Appendix E). The remaining studies assessed various chemical products such as fungicide (García-Cruz et al., 2022), synthetic talc (Glogic et al., 2021), sodium chloride and dechlorinated polyvinyl chloride waste (Lu et al., 2021), biobased aniline (Winter et al., 2021) (Table SI2).

5.3.2.2 Approaches and data sources for prospective scenario modelling

Based on the literature review, we categorized approaches and data sources for prospective scenario modelling for chemical technologies in three main groups:

- Existing scenario narratives/storylines
- Methods for generation of scenarios
- Scenario modelling methods and data sources

Table 5.2 shows three groups of approaches and scenario data sources. Each of these groups includes methods for scenario generation/modelling, as well as sources for scenario data. Description of these methods and scenario data sources are provided in sections 5.3.2.2.1, 5.3.2.2.2 and 5.3.2.2.3.

Table 5.2 *Methods and data sources used for prospective scenario modelling in pLCA.*

	Foreground system		Background system	Examples
	< TRL9	TRL 9		
Existing scenario narratives/storylines, e.g.				
Global narratives and storylines	(X)	(X)	X	SSPs (O'Neill et al., 2014), RCPs (van Vuuren et al., 2011), the International Energy Agency (2024) narratives.
Sector level narratives and storylines, e.g. for chemicals, bulk materials	X	X	X	Scenario narratives/storylines on the development of specific sectors, e.g., chemicals, bulk materials, developed by organizations, companies, and presented in technology roadmaps.
Methods for generation of scenarios, e.g.				
General Morphological Analysis (GMA)	X	X	X	GMA is described in the study of Ritchey (2011).
Scenario-based Inventory Modelling for Prospective LCA (SIMPL)	X	X	X	SIMPL is described in the study of Langkau et al. (2023)
Expert-based approach	X	X		Internally developed scenarios by experts, e.g., LCA practitioners, technology developers.
Scenario modelling methods and data sources, e.g.				

Existing studies	X	X		External studies containing scenario data.
Models		(X)	X	Integrated Assessment Models, the International Energy Agency (2024) models.
Scenario data estimation methods	X			Process simulation, manual calculations, molecular structure models, proxies. A review of these methods can be found in the studies of Tsoy et al. (2020) and Parvatker and Eckelman (2019).
Expert assumptions	X	X	(X)	Scenario data related assumptions made by experts, e.g., LCA experts, technology developers.
Learning curves	X	X		Scenario data (e.g., material and energy efficiencies for the future technologies) can be adapted using learning curves.

"X" = an approach is applicable to an LCA system, "(X)" = an approach is possibly applicable to an LCA system. SSPs = Shared Socio-economic Pathways, RCPs = Representative Concentration Pathways.

Additionally, Table 5.2 illustrates the applicability of methods and scenario data sources for modelling scenarios concerning both the foreground and background systems of chemical technologies. Specifically, certain methods and data sources can be utilized for modelling future scenarios for emerging technologies below TRL9 and/or mature technologies at TRL 9.

5.3.2.2.1 Existing scenario narratives/storylines

Existing scenario narratives/storylines are developed externally by e.g., external experts, external organizations. LCA practitioners intending in modelling prospective scenarios can integrate these external scenarios in their LCA case studies. Two groups of ***Existing scenario narratives/storylines*** can be defined such as ***global narratives and storylines*** and ***sector level narratives and storylines***.

Global narratives and storylines describe possible developments of technologies on the global scale in the future. Examples of these scenario narratives/storylines include Shared Socio-economic Pathways (SSPs) (O'Neill et al., 2014), Representative Concentration Pathways (RCPs) (van Vuuren et al., 2011), and the International Energy Agency (2024) scenario narratives. The review results showed that the studies used data generated by ***models*** (description of models can be found in section 5.3.2.2.3) which in turn are based on ***scenario narratives/storylines***. For example, Wei et al. (2024) modelled the future production volumes of hydrogen production technologies and related technology shares until 2050 based on data from the IEA scenarios (International Energy Agency, 2022, 2021c, 2021a) such as the STEPS, the APS, the NZE scenarios. The data for these scenarios was generated by the IEA's Global Energy and Climate Model (International Energy Agency, 2023b) which was based on the International Energy Agency (2024) narratives. Furthermore, Lamers et al. (2023) used the data of the future energy system scenarios from the model IMAGE (Stehfest et al., 2014) to model background system. This model relied on SSPs (O'Neill et al., 2014) and RCPs (van Vuuren et al., 2011).

Sector level narratives and storylines describe possible future developments of specific sectors, e.g. for chemicals or bulk materials. LCA practitioners can adapt these narratives and storylines from the technology roadmaps of companies and organizations. For instance, Rosental et al. (2020) modelled background scenarios based on the data from the "RESCUE" study (Resource-Efficient Pathways to Greenhouse-Gas Neutrality) (UBA, 2019) of the German Environment Agency. Specifically, they adjusted the production of copper, aluminum, steel, and concrete to an optimized resource extraction and recycling, projected for the year 2050 based on the “RESCUE” study (UBA, 2019).

5.3.2.2.2 Methods for generation of scenarios

General Morphological Analysis (GMA) (Ritchey, 2011) is an example of a method for generation of scenarios. GMA can be defined as “a method for structuring and investigating the total set of relationships contained in multi-dimensional, non-quantifiable, problem complexes” (Ritchey, 2011). The GMA process involves four key steps (Delpierre et al., 2021; Ritchey, 2011): 1) Defining variables, 2) Identifying values for these variables, creating a morphological field, 3) Conducting consistency analysis, and 4) Generating and assessing scenarios. The integration of LCA and GMA is a recently adopted method that has been applied in only a limited number of LCA studies. For instance, Delpierre et al. (2021) applied GMA to generate future possible scenarios for hydrogen production in the Netherlands in 2050.

Scenario-based Inventory Modelling for Prospective LCA (SIMPL) (Langkau et al., 2023) is another method for generation of scenarios. This approach is a stepwise method for a systematic integration of future scenario development into LCA modelling, aligning technology development pathways for both foreground and background systems. The SIMPL approach consists of three steps (Langkau et al., 2023): 1) Identification of relevant inventory parameters and key factors, as well as defines their interrelations; 2) Identification of future assumptions for each relevant parameter and key factor; 3) Combination of assumptions into future scenarios. The SIMPL approach incorporates methods such as PESTEL for identifying scenario factors related to political, economic, sociological, technical, environmental, and legal aspects. It also utilizes causal loop diagrams to visualize interrelations between scenario factors and connect them to the inventory model, as well as cross-consistency assessment to ensure consistency in scenario development. For instance, Del Oso et al. (2023a) used SIMPL approach to generate future possible scenarios for polyhydroxyalkanoates production. It should be noted that ***GMA*** and ***SIMPL*** serve not only as methods for generation of scenarios but also as frameworks for structuring scenarios, facilitating the consistent modelling of both foreground and background scenarios through various methods and data sources outlined in Table 5.2.

Expert-based approach is a method in which scenarios can be developed internally by experts, e.g. LCA practitioners, technology developers. For example, Arvidsson and Molander (2017) developed best-case and worst-case scenarios for upscaling epitaxial graphene production.

5.3.2.2.3 Scenario modelling methods and data sources

Existing studies can contain scenario data suitable for LCA practitioners to use in prospective scenario modelling in their LCA case studies. For example, Valente et al. (2020) used literature technical parameters (e.g., the efficiency values for biomass gasification and steam methane reforming) to model foreground scenarios for hydrogen production for 2030 and 2050.

Scenario data generated by ***models*** have been used by LCA practitioners to model background scenarios for chemical technologies in pLCA. Examples of models include Integrated Assessment Models (IAMs) and the models developed by the IEA. It should be noted that these models are based on ***existing scenario narratives/storylines*** discussed above. For example, IAMs are based on SSPs (O'Neill et al., 2014), while the International Energy Agency (2024) models (e.g., Global Energy and Climate Model) are based on the narratives developed by the International Energy Agency (2024). The reviewed studies used data generated by mostly three models: the studies (Boyce et al., 2024; del Oso et al., 2023b; Lamers et al., 2023; van den Oever et al., 2023) used the data from IMAGE (Stehfest et al., 2014), the studies (Ballal et al., 2023; Watanabe et al., 2022; Wei et al., 2024) applied data from REMIND (Potsdam Institute for Climate Impact Research, n.d.), and the studies used the data from the International Energy Agency (2024) models.

Scenario data estimation methods can be applied as approaches to estimate scenario data. These methods can be combined with ***technology expert consultation*** (a method for generation of scenarios) to form an upscaling method that can be used to upscale an emerging technology. The study conducted by Tsoy et al. (2020) comprehensively reviews upscaling methods applied in ex-ante LCA. Tsoy et al. (2020) proposed a three-step framework for upscaling emerging technology systems in ex-ante LCA. The steps include: (1) Projected technology scenario definition, (2) Preparation of a projected LCA flowchart, (3) Projected data estimation. In this study, upscaling scenarios can be created by developing projected technology scenarios (step 1 of the framework (Tsoy et al., 2020)) using technology expert ***consultation*** and estimating projected data (step 3 of the framework (Tsoy et al., 2020)) by using ***scenario data estimation methods***. In this study, we use the same classification of ***scenario data estimation methods*** as classification of data estimation methods presented in the study of Tsoy et al. (2020). They categorized these methods into four main groups: 1) Process simulation; 2) Manual calculations; 3) Molecular Structure Models (MSMs); 4) Use of proxy. A review of these methods can be found in the studies of Tsoy et al. (2020) and Parvatker and Eckelman (2019).

In this study, the review results showed that most studies used manual calculations (Abbate et al., 2022; Arvidsson and Molander, 2017; Bartolozzi et al., 2020; del Oso et al., 2023b; Delpierre et al., 2021; García-Cruz et al., 2022; Glogic et al., 2021; Günkaya and Banar, 2016; Joyce et al., 2018; Kulkarni et al., 2022; Manda et al., 2015; Müller-Carneiro et al., 2023; Röder et al., 2022; Sirvent et al., 2022), while the remaining used process simulation (Cossutta et al., 2017; da Silva et al., 2021; Delikonstantis et al., 2021; Kanematsu et al., 2021; Lu et al., 2021; Puig-Samper et al., 2022; Thonemann and Maga, 2020; van den Oever et al., 2023; Winter et al., 2021) and proxy (Bartolozzi et al., 2020; Müller-Carneiro et al., 2023). With regards to process simulation, the studies used different process simulation software such as Aspen Plus (Aspentech, 2024), SuperPro Designer (Intelligen, 2020), Multiphase Flow with Interphase eXchange software with a Discrete Element Method solver (Mishra and Rajamani, n.d.), EBSILON Professional (IQONY, 2024), COMSOL Multiphysics (Schlüter and Geitner, 2020). All studies used data estimation methods to estimate material and energy inputs, however, about half of the pLCA studies did not report on emissions data (Table E4 in Appendix E).

Expert assumptions can be referred to a method in which an LCA expert, with or without the involvement of stakeholders, can make assumptions about scenario data. Expert assumptions can be used to model scenarios of future technological development for mature technologies that are at TRL9. For example, Ballal et al. (2023) estimated higher yields from the Fischer-Tropsch synthesis reactor in the foreground system, assuming that there was a 90% recovery of CO_2 emissions from FT synthesis in future scenarios. Currently, on a component level, the Fischer-Tropsch reactor stands at TRL 9.

Also, expert assumptions can be used to model future scenarios for background system. For instance, Cossutta et al. (2017) assumed that decarbonized electricity will be used for the graphene production in the optimistic scenario in the future. In this scenario, they modelled the Norwegian electricity mix as a proxy. Several reviewed studies (Arvidsson and Molander, 2017; Ballal et al., 2023; Cossutta et al., 2017; Delikonstantis et al., 2021; Delpierre et al., 2021; García-Cruz et al., 2022; Rosental et al., 2020; Valente et al., 2020) used expert assumptions method to model future scenarios for foreground and background systems.

Learning curves can be used to model prospective Life Cycle Inventory (pLCI) of a future technology. For example, Lamers et al. (2023) adapted material and energy efficiencies for the future electrolysis technologies using learning curves in pLCA.

Table E4 (in Appendix E) shows the methods and scenario data sources used in the reviewed LCA studies.

5.4 Discussion

In the future, ammonia, methanol, hydrogen, and high-value chemicals are anticipated to play important roles in chemical industry, serving as fundamental components for the synthesis of more complex chemical compounds. Consequently, LCA practitioners intending to carry out pLCA will require pLCA data representing scenarios for the future production of these key chemicals. It is recommended that developers of pLCI databases incorporate these essential chemicals (ammonia, methanol, and high-value chemicals) into their databases, e.g. PRospective EnvironMental Impact asSEment (premise) (Sacchi et al., 2022).

The review findings revealed that among the key chemicals, hydrogen was the most frequently evaluated in pLCA studies. Apart from the studies that assessed the key chemicals, other reviewed pLCA studies mainly focused on polymer materials, nanomaterials, carbon allotropes, and fuels. This could be due to the fact that chemical innovation is primarily focused on substituting conventional fossil-based chemical materials with more sustainable alternatives. For instance, novel bio-based materials may (partially) replace petrochemical products used for producing packaging, automotive components, and aerospace composites (Abbate et al., 2022; Günkaya and Banar, 2016). Novel biofuels and Power-to-X fuels have the potential to be used in shipping, road transport, and aviation (Ballal et al., 2023; van den Oever et al., 2023; Watanabe et al., 2022). Additionally, some of the chemical materials that are being developed and evaluated in pLCA are intended for new applications, such as nanomaterials that can be utilized for producing antibacterial materials (Manda et al., 2015).

We categorized the approaches for modelling future scenarios in chemical technologies into three groups: 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 sources for scenario data. While the reviewed studies employed these approaches to model future foreground scenarios, they often neglected to model prospective background scenarios. However, modelling prospective background scenarios is essential for exploring potential environmental impacts of chemical technologies considering socio-economic factors (Mendoza Beltran et al., 2020). Therefore, it is advisable for LCA practitioners to utilize a combination of foreground and background scenario modelling approaches. To consistently integrate foreground and background scenarios, the ***GMA*** (Ritchey, 2011) and ***SIMPL*** (Langkau et al., 2023) approaches can be applied.

The reviewed pLCA studies that upscaled chemical technology systems estimated material and energy inputs and outputs, however, about half of these studies did not report on the estimation of emissions. This could be due to a lack of comprehensive understanding among LCA practitioners regarding the estimation of emissions in pLCA. Further research is required to address this gap and enhance the knowledge in this area. It may be helpful to explore additional emission estimation methods outside of pLCA studies, such as those used in retrospective LCA or unrelated fields, e.g. chemical engineering and risk assessment. For instance, machine learning methods such as Classification and Regression Tree (CART) (Meyer et al., 2019), Random Forest (RF) (Meyer et al., 2019; Ye et al., 2022), Support vector machine

(SVM) (Ye et al., 2022), Extreme gradientboosting (XGBoost) (Zhao et al., 2021) have been used to estimate emissions. Hou et al. (2018) proposed another computational approach to predict data, including emissions, named as similarity-based link prediction. Possibly, these machine learning methods could be used to estimate emissions in pLCA.

Our review focused on approaches used to model prospective scenarios of chemical technologies in the LCI phase. Therefore, we did not include studies on prospective impact assessment methods as they do not focus on LCI modelling. However, there are various prospective impact assessment methods used in the chemical field. Machine learning methods have been used in prospective impact assessment of chemical technologies. For example, Kleinekorte et al. (2023) presented a framework called *A PROcess-specific, PRedictive impact AssessmenT method for Emerging chemical processes (APPROPRIATE)*, which allows for process-specific prediction of the global warming impacts of organic molecules (Kleinekorte et al., 2023). Sun et al. (2023) performed data processing using a feature selection method and weighted Euclidean distance. Based on the data processing, they developed artificial neural network (ANN) models for predicting the life-cycle environmental impacts of chemicals. Kleinekorte et al. (2020) reviewed papers that predicted life cycle impacts of chemicals based on their molecular structure. Karka et al. (2022) presented a data-science based framework which can be used to estimate LCA metrics of bio-based processes in early design stages.

This study has some limitations that are important to note. Firstly, there is a possibility that certain pLCA studies may have been overlooked during the literature search as the keywords utilized in the Web of Science search might not have captured all relevant studies. Consequently, some approaches for modelling prospective scenarios may have been missed during the literature search. However, we believe that our literature review did identify the most often used approaches for scenario modelling in pLCA. Secondly, it is worth mentioning that Table 5.2, which outlines the approaches for modelling prospective scenarios, may require updating in the near future. Given the rapid development of the pLCA field, new studies frequently introduce novel approaches, necessitating periodic revisions to incorporate these advancements.

5.5 Conclusion

The objective of this study was to determine chemicals that would play a key role in the future chemical industry. Furthermore, we aimed to identify prospective scenario modelling approaches that could be used to model future scenarios of these key chemicals. In this section we provide answers to the sub-questions and the main research question presented at the beginning of the study.

1. What are the key chemicals that are expected to play an important role in the future, and what are their potential future production routes?

The first sub-question was addressed by reviewing reports and roadmaps on climate change mitigation strategies in the chemical industry. As a result, the chemicals such as ammonia, methanol, and high-value chemicals were identified as key chemicals that would play an important role in the future chemical industry. In addition, hydrogen was identified as a key chemical as it is expected to be used in the future production of ammonia and methanol. Currently, the key chemicals (ammonia, methanol, and high-value chemicals) are fundamental in the production of thousands of other chemicals and account for almost two-thirds of the total energy used by the chemical sector. These key chemicals are expected to maintain their essential role in the chemical industry in the future since they will continue to serve as the primary building blocks for more complex chemicals like polymers, agrochemicals, and specialty chemicals and will thus be in high demand.

Different roadmap scenarios have varying expectations regarding the future production routes of the key chemicals such as ammonia, methanol, and high-value chemicals. For ammonia production, the Haber-Bosch process is expected to remain the main technology in the future, while hydrogen production routes for ammonia will differ across scenarios. It is projected that there will be an increase in gas-based production with CCS and electrolysis and a decrease in fossil-based production without CCS in 2050 compared to 2020. For methanol production, in general, it is expected that there will be a shift from coal-based production to natural gas-based production in 2050. Regarding high-value chemicals production, roadmap scenarios expect that naphtha steam cracking and ethane steam cracking will remain to be the dominant production routes in 2050. However, an increase in share for naphtha catalytic cracking and "Methanol to olefins/aromatics" route is expected in 2050 compared to 2017.

2. Which of the key chemicals identified have been assessed using pLCA? Additionally, for which other chemicals have pLCAs been conducted?

The second sub-question of the study was addressed by reviewing pLCA studies. The review results showed that hydrogen was the most frequently assessed among key chemicals. Apart from key chemicals, other chemicals that were assessed in pLCA included polymer materials, nanomaterials, carbon allotropes, and fuels. One possible explanation is that chemical innovation primarily targets replacing traditional fossil-based chemical materials with more sustainable alternatives. For example, bio-based materials may (partially) replace petrochemical products for e.g., packaging, Power-to-X fuels and biofuels may replace fossil-based fuels. Furthermore, certain chemical materials undergoing development and assessment in pLCA are designed for new applications, such as nanomaterials used for the production of antibacterial materials.

3. What can be learned from existing pLCA studies of the key chemicals? Additionally, which methods are available from pLCAs of other chemicals that could be applied to model key chemicals?

Regarding the third sub-question, we classified the approaches for modelling future scenarios in chemical technologies into three main groups: 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 sources for scenario data.

Certain methods and scenario data sources are applicable to foreground scenario modelling, others to background scenario modelling, and some to both. These methods and scenario data sources from different groups can be combined to model a future scenario for a chemical technology. While reviewed studies mainly focused on foreground scenarios, they often neglected modelling prospective background scenarios. However, incorporating these scenarios is crucial for assessing potential environmental impacts of chemical technologies in light of socio-economic factors.

Reviewed studies utilized the data estimation methods for upscaling emerging technologies such as manual calculations, process simulation, and proxy. They applied these methods to estimate material and energy flows. However, about half of the pLCA studies did report on emissions data. Therefore, it may be beneficial to explore additional emission estimation methods beyond pLCA studies, such as those utilized in retrospective LCA or unrelated fields like chemical engineering and risk assessment.

The main research question: Which approaches are available to model future foreground and background scenarios for key chemicals in pLCA?

The review study identified various approaches applied in pLCA studies to model prospective scenarios. We categorized these approaches into three main groups 1) Existing scenario narratives/storylines, 2) Methods for generation of scenarios and 3) Scenario modelling methods and data sources. Within each of these groups, there are methods for generating and modelling scenarios and sources for scenario data. Some methods and scenario data sources are suitable for modelling foreground scenario modelling, others for modelling background scenarios, and some are applicable to both types of scenarios.

Additional research is needed to determine if there are limitations to the applicability of the existing scenario modelling approaches to certain chemical technologies, e.g., nanomaterials, polymer materials, fuels. There could be the case that some approaches are only suitable to one type of chemical technology and not be suitable for another type. However, conducting such research is currently challenging due to the limited availability of pLCA studies providing comprehensive information on approaches and their applications. Therefore, pLCA practitioners should conduct more LCA studies of chemical innovations providing more examples to facilitate this research.

As it was noted above, there are relatively few pLCA studies focusing on new chemical technologies. Consequently, there is a possibility that the existing approaches to prospective scenario modelling, as outlined in this study, might not be directly applicable to chemical innovations that have not been assessed yet. Therefore, LCA practitioners would need to either create new approaches to evaluate such technologies or modify existing approaches.

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