LCA of Chemicals and Chemical Products

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Chapter 31
LCA of Chemicals and Chemical Products

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Abstract This chapter focuses on the application of Life Cycle Assessment (LCA) to evaluate the environmental performance of chemicals as well as of products and processes where chemicals play a key role. The life cycle stages of chemical products, such as pharmaceuticals or pesticide active ingredients, are discussed and differentiated into extraction of abiotic and biotic raw materials, chemical synthesis and processing, material processing, product manufacturing, professional or consumer product use, and finally end-of-life treatment. LCA is put into perspective of other chemicals management frameworks and concepts including risk assessment, green and sustainable chemistry, and chemical alternatives assessment. A large number of LCA studies focuses on contrasting different feedstocks or chemical synthesis processes, thereby often conducting a cradle to (factory) gate assessment. While typically a large share of potential environmental impacts occurs during the early product life cycle stages, potential impacts related to chemicals that are found as ingredients or residues in products are dominated by the product use stage. Finally, methodological challenges in LCA studies in relation to chemicals are discussed from the choice of functional unit, over defining the system boundaries, quantifying emissions for many thousand marketed chemicals, to characterising these emissions in terms of toxicity and other impacts, and finally interpreting chemical-related LCA results. The chapter is relevant for LCA students and practitioners who wish to gain basic understanding of LCA studies of products or processes with chemicals as a key aspect.

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31.1 LCA and Chemicals: Introduction and Context

31.1.1 Chemicals and Their Relevance in Society

Chemicals are everywhere. Almost every second a new entry is added to the list of more than 100 million unique chemicals and substances registered in the Chemical Abstracts Service (CAS; www.cas.org), the world's authority on chemical information. Since industrialisation, the welfare of modern society largely builds on extensively mining minerals and fossil fuels including coal, petroleum and natural gas to produce large quantities of synthetic chemicals ('synthetic' simply means man-made and should not be confused with 'artificial', which implies that a chemical does not occur naturally). Consequently, the enormity and diversity of the chemical industry is astounding and poses various challenges for the management of environmental and human health impacts related to chemicals production and use. In this chapter, we outline important aspects to know about chemicals in the context of LCA.

Fundamentally, chemicals are substances composed of one or more atoms, and make up every material thing on earth—including our bodies. The atomic composition of chemicals classifies them essentially as 'organic' (chemicals with molecules built on a skeleton of interlinked carbon atoms and primarily consisting of carbon, oxygen, and hydrogen) and 'inorganic' (chemicals with molecules generally lacking carbon-to-carbon bonds, but instead based on the rest of the elements, including metals). In this sense, 'organic' has nothing to do with 'organic food' or 'organic farming' or 'organic lifestyle' as these terms generally refer to promoting sustainability. The atomic composition, molecular structure and ionisation (positive/negative charge) all influence chemical reactivity and behaviour in the environment as well as in living organisms. Because of this, chemical behaviours can be predicted and tested, and chemicals can be designed by industries to fulfil biological (e.g. medical) and physical (e.g. solvent) functions.

Chemicals may also be classified according to functional groups (e.g. alcohols, amines, acids and bases), structural groups (e.g. polycyclic aromatic hydrocarbons), physical structure (e.g. nanotubes), feedstock sources (e.g. petrochemicals derived from fossil fuels, biochemicals derived from starch- and sugar-based feedstocks), physicochemical properties (e.g. volatile, lipophilic), use function (e.g. surfactants, warfare agents), means of creation (e.g. reaction intermediates, metabolites), main economic sector (e.g. cosmetics, agrochemicals), toxicity endpoints (e.g. carcinogens, neurotoxins, endocrine disruptors), and other aspects.

Established nomenclatures or patent names can be used to name chemicals. Most chemicals have an assigned CAS Registry Number except some metabolites of natural processes or grouped chemicals such as polychlorinated dibenzofurans. CAS numbers are the most discriminant method for chemical reference. Of the chemicals registered by CAS, more than ten thousand are currently in commercial use, some with annual production volume of millions of tonnes, while most chemicals are produced at less than thousand tonnes per year. Worldwide, the production of chemicals has risen to several hundred million tonnes per year and sales were valued in 2013 at 3156 billion Euro with an average annual growth of 10.3% between 2003 and 2012 (CEFIC 2014). China dominates world chemical sales with a share of 33.2% followed by the European Union (16.7%), USA (14.8%), and Japan (4.8%) in 2013.

Over the last decades, there has been a shift in global chemicals production. As an example, polychlorinated biphenyls (PCBs) have been replaced by chlorinated paraffins in various applications. While PCBs have been primarily produced in USA and Europe with a total historical production volume of 1.3 million tonnes between 1930 and 1995, chlorinated paraffins are almost exclusively produced in China and reach production volumes of more than one million tonnes per year (Fantke et al. 2015). Databases, such as the European Chemicals Agency (ECHA) Registered Substances database (echa.europa.eu/information-on-chemicals), the Household Product Database (householdproducts.nlm.nih.gov), Hazardous Substances Data Bank through ToxNet (toxnet.nlm.nih.gov), and the Chemical and Product Categories Database (actor.epa.gov/cpcat/) attempt to keep track of chemicals, their uses, properties and/or toxicity, but large data gaps still remain.

The chemical and pharmaceutical industries are a major driver of the welfare of modern society and scientific progress. These industries rely on the extraction, purification and synthesis of both naturally occurring and synthetic chemicals and are among the largest and most influential economic sectors at the global scale. Main production segments are petrochemicals (e.g. benzene, styrene), consumer chemicals (e.g. detergents, fragrances and flavours), speciality chemicals (chemicals used for providing a special performance or effect, e.g. paints, dyes, adhesives), basic inorganics (fertilisers, industrial gases like nitrogen and oxygen), and polymers (e.g. plastics, synthetic rubber and fibres). One of the largest segments is the production of organic chemicals with, e.g. formaldehyde, aromatics, acids, alcohols and esters providing the building blocks for drugs, agrochemicals, cosmetics and many other applications.

Along with societal advantages, the rise of chemical industries has also caused various undesirable consequences. Health impacts of air pollution are increasing worldwide and there is currently insufficient information to fully assess the impacts of chemicals on humans and the environment. Rachel Carson's book *Silent Spring* published in 1962 documented the detrimental impacts of chemicals on wildlife and humans, especially related to using synthetic organic pesticides, and marked a major change in public awareness that eventually inspired regulation of industry and for example the creation of the United States Environmental Protection Agency. Since that time, a remarkable amount of research correlates and demonstrates impacts on human and ecosystem health as well as the environment (e.g. the ozone layer) caused by intentional and unintentional chemical releases both indoors and outdoors. Some reported impacts are directly related to the chemical industry, whereas other impacts are related to the use or disposal of chemicals by other industries. In the following sections, we overview strategies for chemical management, focusing particularly on life-cycle assessments of chemicals production processes and chemical products.

31.1.2 Chemicals Management in Relation to LCA

Depletion of the ozone layer by chlorofluorocarbons used as refrigerants and solvents, soil and water pollution with heavy metals from ore mining and processing, pesticide emissions and residues in food, the formation of dioxins by incomplete combustion processes, and leaching of fertilisers into groundwater are just examples of the many problems associated with chemical releases to the environment. Hence, managing human and environmental risks posed by chemicals that are potentially toxic or may lead to other impacts is a major concern of regulators, industries, consumers and other stakeholders. As a consequence, the chemicals industry is one of the most regulated industries with main focus on regulating chemicals in consumer products and minimising chemical emissions to the indoor (workplace, public buildings and household) and outdoor environments along product life cycles. In the context of chemicals management, risk is defined as the probability of a chemical to cause an adverse effect (hazard) occurring as a result of a given contact between the chemical and humans or the environment (exposure). In reality, risks associated with chemical emissions from a given product or process can arise at specific points in space and time and depend on chemical background concentrations due to all release sources. In LCA, information on emission location and time as well as information on background concentrations, e.g. from sources outside the considered product system, is usually not available. Hence, modelled impacts in LCA are not interpreted in terms of actual risk, i.e. real environmental effects, but in terms of 'potential impacts' (Chap. 10) used as environmental performance indicators for comparing and optimising products or systems with respect to a defined functional unit (Hauschild 2005). However, models applied in LCA can also be advanced and adapted to consider background concentrations as well as spatiotemporal resolution (e.g. daily or seasonal changes), and in such cases estimated potential impacts can be interpreted as estimates of actual risk.

Chemicals management occurs from local to global scale, from specific product–chemical combinations to entire industries and from raw material acquisition to waste handling, depending on the intended scope and purpose. The Montreal Protocol on Substances that Deplete the Ozone Layer (ozone.unep.org) and the Stockholm Convention on Persistent Organic Pollutants (POPs; www.pops.int) are examples of global chemicals management treaties, whereas the Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) is a recent example of an international legislative framework for managing industrial chemicals in the European Union. At all levels and scopes, effective chemicals management relies on assessment tools and guiding principles to ensure consistency and the achievability of defined goals. There are many examples of chemicals assessment tools and guidance, such as risk assessment, green and sustainable chemistry, chemical alternatives assessment, life cycle assessment, and a market for entrepreneurs to create industry-specific interfaces and applications. In the following sections, risk assessment (Sect. 31.1.3), green and sustainable chemistry

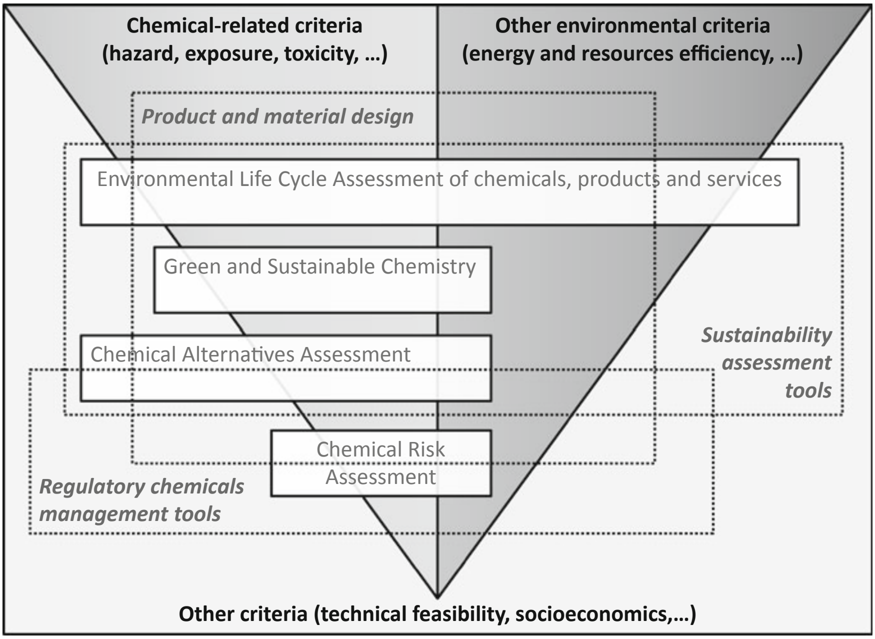


Fig. 31.1 Conceptual relationships of main chemical management tools

(Sect. 31.1.4), and chemical alternatives assessment (Sect. 31.1.5) are discussed as commonly used chemical management tools that have both complementary and overlapping aspects with LCA as illustrated in Fig. 31.1.

31.1.3 Risk Assessment and Safety

Chemical risk assessment—also referred to as chemical safety assessment—is implemented in various regulatory frameworks and is one of the most widely used chemicals management tools. Risk assessment (‘*How risky is a situation*?’) as an integral part of risk management (‘*What shall we do about it, if a situation is risky*?’) essentially emerged at the start of the nineteenth century from studying hazards and risks associated with different occupations. Risk assessment mainly consists of hazard identification, dose-response assessment, exposure assessment and risk characterisation. Depending on the context, ‘risk’ and ‘safety’ have different meanings with regulatory policy commonly seeking to minimise risk while optimising safety. In this context, risk is generally defined as the probability of harm, whereas safety is described as the absence of harm (Embry et al. 2014).

Chemical ‘safety’ is defined by legislators or regulators and can vary from country to country and evolves over time as science progresses. In this sense, ‘safe’ is not synonymous with 'natural' as it is often perceived. In fact, using the word 'natural' is misleading in the context of chemical safety (and LCA) and there are many naturally occurring chemicals that have very harmful properties like arsenic, nicotine or radon. As a consequence, we need to acknowledge that it is not always the 'natural' chemicals or solutions that are most 'environmentally friendly'—a common misconception in different science-policy fields and among consumers. Defining safety *thresholds*, e.g. chemical concentrations in different environmental media (e.g. ambient air, soil, water) or in food, is a common strategy in chemical risk assessment, and generally refers to levels below which a risk is considered 'safe' by a risk manager, meaning that any risk below threshold is regarded as 'acceptable'. As an example, chemical exposure resulting in one additional cancer case or less over lifetime in a population of one million people is regarded as an acceptable risk, i.e. safe, in the U.S. (van Leeuwen and Vermeire 2007). Using units like 'part per million' (ppm) as in one cancer case in a million or 'part per billion' is common for describing (very small) amounts of chemicals in the environment. To get an impression of how much one ppm actually is, we can use 1 teaspoon of salt (5.5 g) in 5.5 tonnes of potato chips corresponding to one part of salt per one million parts of potato chips.

Thresholds are also applied when managing environmental systems and for developing chemical pollution control strategies, such as allowable nutrient releases from wastewater treatment plants or setting greenhouse gas emission targets, or in the context of 'planetary boundaries' in an attempt to assess if the pressure from chemical pollution (analogous to the amount of receiving environment required to dilute pollution to a threshold level) exceeds a planetary boundary (analogous to the amount of receiving environment available) for a 'safe operating space' for human activities (MacLeod et al. 2014). Chemical pollution levels have recently been expressed as 'chemical footprints' that can be compared with respective planetary or other boundaries for chemical pollution (Posthuma et al. 2014) to assess how companies or nations perform with respect to different chemicals management issues.

Risk assessment approaches take a receptor perspective (Fig. 31.2, right-side box), where thresholds are set in order to protect specific receptors, i.e. exposed humans or ecosystem species. In a receptor perspective, all relevant sources of a chemical or target chemicals are typically considered. In contrast, impact assessment tools in LCA are generally not receptor-oriented or threshold-based. This is because LCA takes a 'producer' (or 'emitter') perspective (Fig. 31.2, left-side box) by comparing potential impacts relative to each other across compared products and life cycle stages, aiming at minimising impacts considering various receptors (entire human populations, freshwater ecosystems, marine ecosystems, etc.). Differences and commonalities of risk assessment and LCA have been contrasted elsewhere (e.g. Bare 2006; Pennington et al. 2006), and there are several attempts combining, blending or integrating both concepts (Harder et al. 2015).

An increasing number of chemicals is approved for use in commerce, e.g. in food contact materials, but often lacks adequate information to characterise risks (Neltner et al. 2013). In response, high-throughput screening ('first tier'

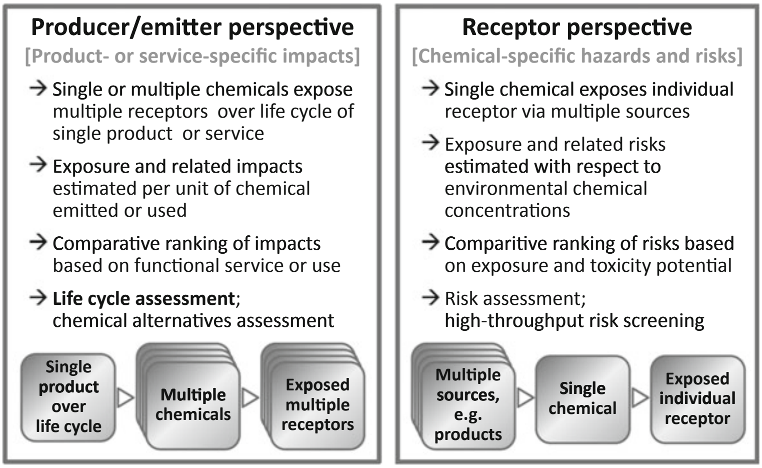


Fig. 31.2 Examples and underlying characteristics of dichotomous perspectives followed in different chemicals management approaches

assessments) of chemical risks has emerged as a strategy for prioritising and ranking chemicals for more in-depth study ('higher-tier' assessments). First-tier screening usually relies on ranking chemicals with respect to hazard (e.g. chemical toxicity) combined with estimates of exposure. 'High-throughput' refers to processing dozens to thousands of chemicals via resource efficient methodologies, such as robotic in vitro bioassays (instead of animal in vivo experiments) and low-tier computational models relying on databases (instead of data-intensive complex and time-consuming modelling). LCA impact assessment models have been used in high-throughput risk screening offering dual purpose and a promising area of interdisciplinary overlap to manage chemical risks (e.g. Shin et al. 2015).

31.1.4 Green and Sustainable Chemistry

'Green chemistry' is a concept that was coined by the U.S. Environmental Protection Agency in the early 1990s in response to the Pollution Prevention Act and increasing attention to chemical pollution. This concept builds upon a set of 12 Principles of Green Chemistry defined by Anastas and Warner (1998) aiming at reducing or eliminating hazardous substances in the design, manufacture and application of chemical products. Thereby, 'green' refers to more environmentally benign (less hazardous) chemicals. The concept of 'sustainable chemistry' is broader than the scope of green chemistry and strives towards 'eco-efficiency'. In addition to chemical hazards, sustainable chemistry centrally focuses on optimising the use of finite resources, while reducing environmental impacts of chemical production (OECD 2012). Sustainable chemistry—sometimes also referred to as sustainable chemistry and engineering—is rooted in the concept of Sustainable Development established in Rio de Janeiro in 1992 at the United Nations Conference on Environment and Development and are guided by 9 Principles of Green Engineering postulated at the Sandestin conference (Abraham and Nguyen 2003).

Green and sustainable chemistry are concepts focusing on the technological approaches aiming at the reduction of resource consumption and pollution prevention in chemical production processes rather than focussing on the assessment of chemicals in the environment. Hence, green and sustainable chemistry—often relying on comparing qualitative or semi-quantitative indicator results—are primarily applicable in the design phase of products to guide innovation and to support sustainable production goals.

Green chemistry in relation to LCA has been discussed in more detail elsewhere (e.g. Anastas and Lankey 2000). In summary, compared to green and sustainable chemistry, LCA aims at fully quantifying potential impacts associated with a chemical product or production system over its entire life cycle. Using LCA in early stages of chemical product and process design of various sectors including emerging technologies (e.g. bio- and nanotechnology) has provided insight into the relationship between chemical and process parameter selection and related impacts on humans and the environment (Kralisch et al. 2015). LCA results have moreover demonstrated that quantitative methods are needed to assess the environmental performance of 'green' chemicals (Tufvesson et al. 2013). This is especially relevant as green chemistry usually focuses on optimisation of (production) processes, including some specific end-of-life problems related to chemicals, which may still risk sub-optimisation when a full life cycle perspective is lacking.

Using LCA in early product development stages, for example before a product has been created and marketed, comes with methodological and practical challenges, such as low data availability, uncertainty related to future product applications, and unclear scale of production for a changing market. Therefore, LCA has mostly been applied to chemical products and processes that are already well established and operational at the market scale, which leads to LCA results often being reactive instead of proactive.

31.1.5 Chemical Alternatives Assessment

Chemical alternatives assessment (CAA) aims to identify, compare and select safer alternatives to substitute (replace) harmful chemicals in materials, processes and products on the basis of their hazards, performance and economic viability (Hester and Harrison 2013). CAA emerged from the U.S. Environmental Protection Agency's Design for Environment (DfE) program in the late 1990s to promote less hazardous chemicals in various products and applications, and to avoid unintended consequences of harmful alternatives resulting in incremental improvements or even 'regrettable substitution' situations (Fantke et al. 2015). Ideally, CAA tools would evaluate hazard, exposure, life cycle and social impacts, economic feasibility and technical performance of alternative solutions, and consider chemicals, materials, products or technologies, and behavioural changes as viable solutions options. In reality, however, most CAA tools focus only on comparisons of hazard scores and exclusively consider chemicals as potential solutions. Several existing CAA tools have been compiled into the OECD Substitution and Alternatives Assessment Toolbox (www.oecdsaatoolbox.org).

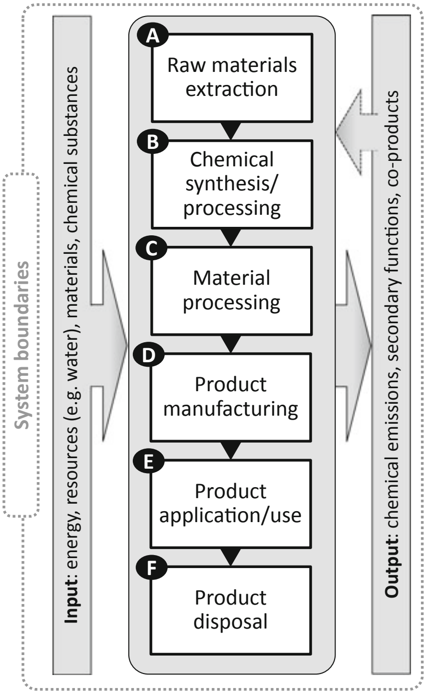
The concept of 'acceptable risk' (as applied in risk assessment) is usually avoided in CAA in order to support selecting *relatively* less hazardous chemicals and materials in products (Whittaker 2015). Despite the current focus on assessing chemical hazard, including exposure, life cycle, and social considerations are lately also gaining more attention (Jacobs et al. 2016), focusing the CAA discussion around using more quantitative and chemical function-based methods and tools (Tickner et al. 2015). However, the need for rapid screening of numerous viable alternative solutions prevents CAA from simply adopting the use of LCA tools due to high complexity and data demand.

CAA is mainly used to identify and evaluate solutions to hazardous chemicals in products that have been targeted for phase-out, and to inform early product development to minimise reliance on hazardous chemicals. With that, CAA takes the 'producer' perspective similarly to LCA (Fig. 31.2, left-side box), focusing on the impact of chemicals and their alternatives on various receptors. The main difference between CAA and LCA is that while CAA focuses on seeking for viable alternatives to harmful chemicals, LCA considers the life cycle of whole products or processes not focusing specifically on the content of one or more chemicals that might be considered 'hazardous', but instead evaluating the overall product or process environmental performance.

31.2 LCA Applied to Chemicals

Chemicals play a central role in the LCA framework for different reasons. Hundreds of chemical emission (inventory) flows typically occur along the life cycle of products or systems (Fig. 31.3) and are quantified as part of the Life Cycle Inventory (LCI; see Chap. 9) phase. Chemicals are also often precursors of product materials, and input for manufacturing and disposal processes. Chemical emissions associated with energy conversion during manufacturing, transport of goods and end-of-life treatment processes often dominate overall emission profiles for many product categories resulting in potential environmental impacts that can be characterised in the Life Cycle Impact Assessment (LCIA; see Chap. 10) phase.

Chemicals contribute to nearly all LCIA impact categories affecting human health and ecosystem quality as two main areas of protection in LCA, with resources (e.g. water) being an area that is usually not relevant for chemicals (Hauschild et al. 2013). In LCIA, chemicals contribute to global warming, stratospheric ozone depletion, formation of photochemical ozone in the troposphere, air



Relevant questions for different life cycle stages…

A: Fossil or bio-based resources; virgin or recycled materials; alternative use of resource or material (e.g. food) or waste (e.g. shell or husk); location of extraction (e.g. rain forest, ocean, conflict zone); secondary functions (e.g. algae waste treatment)?

B: Reactor configuration (e.g. batch or continuous); number of reaction steps or unit operations; solvents; catalysts (e.g. enzymes, rare metals)?

C: Machine lubricants; chemical contents and concentrations?

D: Machine lubricants; solvents; adhesives?

E: Product longevity; secondary functions; exposure during use; nature of use (e.g. amount used; additional requirements such as hot water); societal function (e.g. to cure a disease)?

F: Special handling (e.g. pharmaceuticals); disposal location; process (e.g. incineration or landfil); reuse opportunity; circularity of waste streams?

A-D and **F:** Waste handling (e.g. municipal or industrial; type); co-products (e.g. materials; energy from incineration); existing or new infrastructure; efficiency; worker exploitation or occupational exposure?

Fig. 31.3 Generic life cycle stages and system boundaries for chemical products or materials and LCA-related questions. In some cases, chemical processing may be followed by material production (e.g. polymers) before manufacturing a product (e.g. plastic bottles), while in other cases, chemicals (e.g. solvents) may be directly added to products or product manufacturing processes. *Underlined topics* are mostly lacking methods or not included in environmental LCA studies

pollution (via respiratory particles and precursors), aquatic and terrestrial acidification and eutrophication, and last but not least human toxicity and aquatic and terrestrial ecotoxicity. Only a handful of chemicals are associated with the majority of abovementioned impact categories, such as carbon dioxide, methane and other greenhouse gases contributing to global warming impacts or ammonia, nitrogen oxides, phosphate and some other nitrogen and phosphorus containing chemicals contributing to aquatic eutrophication. In contrast, thousands of chemicals can be characterised as potentially toxic to humans and/or ecosystems (Rosenbaum et al. 2008). This is, however, only a small fraction of the tens of thousands of commercially relevant chemicals.

The generic life cycle stages shown in Fig. 31.3 are applicable to a chemical product (e.g. pharmaceutical or dye) or material (e.g. polymer), from raw materials extraction to product disposal, often referred to as ‘cradle to grave’ (Fig. 31.3, stages A–F). A ‘cradle to grave’ LCA study can provide valuable insight regarding which stages dominate the impacts throughout a product life cycle. Some of these life cycle stages, however, may not be relevant depending on the goal (Chap. 7) and scope (Chap. 8), and the product system under study. For example, the 'material processing' stage may not be relevant in cases where a chemical is directly added into a product as an ingredient, such as fragrances in cosmetics or detergents in cleaning products. As another example, the 'product application/use' or 'product disposal' stages may not be relevant for comparing the environmental performance of chemical synthesis or production processes as long as the compared processes do not influence the chemical amount used in a product or for product disposal.

An LCA study from raw material extraction to chemical product manufacturing, i.e. without considering product use and disposal stages, is referred to as 'cradle to gate' (Fig. 31.3, stages A–D), which refers to the 'gate' of the manufacturing or production facility (which could be the 'gate' of a chemical or product 'factory', depending on the focus of the study). In Table 31.1, different assessment scopes for LCA studies focusing on chemicals in materials, products and processes are contrasted and associated with relevant chemicals management questions.

LCA can help identify a variety of impacts associated with chemical production, use, and disposal, that are either intrinsic to a chemical (e.g. toxicity potential) or related to supporting industrial chemical processes (e.g. water consumption, greenhouse gas emission). The main uses of LCA for managing chemicals and chemical processes are to compare impacts between products or services, or to identify 'hot spots' within a life cycle that contributes greatly to the impacts of a product or service. With respect to chemicals, LCA can be applied to various combinations of the generic life cycle stages in Fig. 31.3 depending on the LCA study goal and chosen system boundaries. In some cases, individual life cycle stages and associated inputs or outputs may be skipped or not considered important for the defined system. The chemical industry developed a guidance document to support the assessment of the environmental performance of chemical products based on attributional LCA, i.e. referring to process-based modelling and excluding market-mediated effects (WBCSD 2014).

In the following sections, an overview is given of how LCA has been applied to consider these various life cycle stages and the general lessons learnt from these studies. Thereby, LCA can be used to compare impacts at the level of chemicals in materials, products and formulations or at the level of chemical synthesis and production processes.

31.2.1 Chemicals in Materials, Products, and Formulations

A subset of materials, products, formulations (combination or mixture of chemicals) and processes are intrinsically reliant on the functionality of key chemical ingredients. In this section, main trends are summarised in using LCA- or LCA-based methodologies. This may include also partial LCA studies, e.g. methods only considering a subset of life cycle stages (i.e. cradle to gate or gate to gate), with focus on chemicals in materials, products and formulations.

Table 31.1 Relevant life cycle assessment scopes and life cycle stages for selected chemicals management questions and example studies

Chemicals management questions	Assessment scopes and considered life cycle stages	Example studies
What is the environmental performance of different products with respect to chemical emissions?	• Cradle to grave • Stages A–F (Fig. 31.3) • Focus on chemicals consumption and emissions	• Cleaning products (Van Lieshout et al. 2015) • Textiles (Roos et al. 2015)
What are the environmental profiles of the production of different chemicals?	• Cradle to (factory or consumer) gate • Stages A–D or a subset of these stages (Fig. 31.3) • Focus on chemical manufacturing	• Pharmaceuticals (Wernet et al. 2010)
Which life cycle stage of a chemical product life cycle contributes most to environmental impacts?	• Cradle to grave • Hotspot analysis including stages A–F (Fig. 31.3) • Focus on chemicals as products	• Plant protection products (Geisler et al. 2005)
Which chemical synthesis and/or manufacturing processes contribute most to environmental impacts?	• Cradle to (factory) gate • Hot-spot analysis including stages A–B or A–C (Fig. 31.3) • Focus on chemical manufacturing	• Pharmaceuticals (De Soete et al. 2014) • Nano-materials (Pati et al. 2014)
Which life cycle stage of a chemical in a product contributes most to human exposure?	• Cradle to grave • Partial LCA (only human e.g. exposure estimates) including stages A–F (Fig. 31.3) • Focus on chemicals in products	• Cosmetics (Ernstoff et al. 2016a)
Which feedstock provides the most environmentally friendly substrate for biochemical synthesis?	• Cradle to (factory) gate • Stages A or A–B (Fig. 31.3) • Focus on chemicals and raw materials consumption	• Acrolein (Cespi et al. 2015) • PET (Akanuma et al. 2014)

LCA studies have focused on pharmaceuticals (e.g. De Soete et al. 2014), cleaning products (e.g. Van Lieshout et al. 2015) and pesticide formulation products (e.g. Geisler et al. 2005) as examples of products where chemicals provide the main product functions. Other LCA studies on chemicals with in-product functions include studies focusing on flame retardants in electronics (Jonkers et al. 2016), nano-materials used in bandages and cosmetics (Botta et al. 2011), and polymers used in food packaging (Hottle et al. 2013). Chemicals required for industrial processes have also been assessed in LCA studies, including industrial solvents (Zhang et al. 2008) and chemicals used for the production of treated water, oil and

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gas, printing paper and dyed textiles (e.g. Alvarez-Gaitan et al. 2013; Parisi et al. 2015).

When analysing LCA studies on chemical-based functions, a few generalisations emerge. For example, it is important to consider life cycle thinking early on in the design phase of products and processes whenever possible and it has been shown that simplified tools may help in this process (e.g. De Soete et al. 2014). Furthermore, it has been demonstrated that hybridised LCA tools or metrics can be useful to improve communication and management for specific stakeholders (e.g. Alvarez-Gaitan et al. 2013).

Several LCA studies indicate that being sceptical of services deemed ‘green’ or ‘sustainable’ is crucial, especially when an LCA has not yet been performed. Case studies on, e.g. ‘green’ solvents (Zhang et al. 2008) or ‘sustainable’ bio-based chemicals and materials (e.g. Hottle et al. 2013) demonstrate that materials and products guided by principles of ‘sustainability’, ‘eco-friendliness’ or ‘green chemistry’ can have significant, but often disregarded or unassessed, environmental impacts. An example is given in Fig. 31.4, where environmental life cycle impacts of petro- and bio-based polymers are contrasted based on data from Hottle et al. (2013).

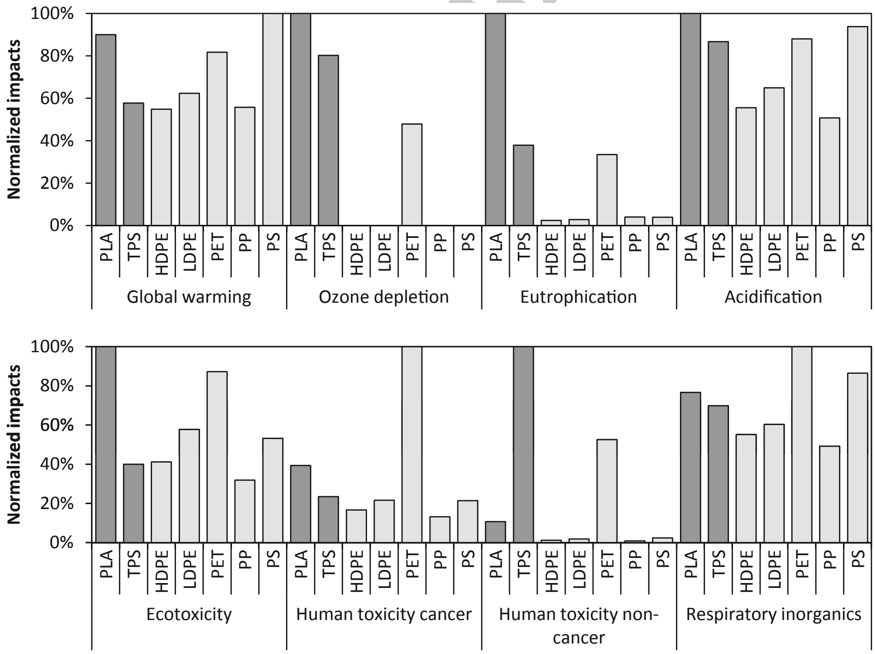

Fig. 31.4 Impact scores for LCAs of two bio-based polymers (*dark bars*; *PLA* Polylactic acid, *TPS* Thermoplastic starch) compared to petroleum-based polymers (*light bars*; *HDPE* High-density polyethylene, *LDPE* Low-density polyethylene, *PET* Polyethylene terephthalate, *PP* Polypropylene, *PS* Polystyrene) per kg of produced granule, normalised for each category to the polymer with highest impacts (based on data from Hottle et al. 2013)

According to this study, bio-based polymers lead to higher impacts than petro-based polymers for several impact categories, which contradicts assumptions that bio-based automatically implies 'green' or 'sustainable' (see also Chap. 30). Higher impacts for bio-based polymers are mainly associated with feedstock-related agricultural emissions of fertilisers (eutrophication) and pesticides (human toxicity and ecotoxicity), as well as deforestation (impacts related to changes in land use). However, the relative importance (i.e. contribution to overall environmental impacts) of the different impact categories also needs to be considered when evaluating the overall environmental performance of different polymers or other chemical products and processes.

Often products are referred to as 'green' or 'sustainable' based on a single environmental issue (e.g. reducing greenhouse gas emissions), or based on following the principles of green chemistry in chemical design only. However, chemical products that are claimed to be 'green' or 'sustainable' may in fact lead to greater impacts on the environment or humans than the conventional alternatives. For example, 'eco-friendly' food packaging made of plant fibres may increase exposure and environmental emissions of highly hazardous fluorinated chemicals (Yuan et al. 2016), and 'green' solvents can have higher impacts across many impact categories when compared to conventional solvents (Zhang et al. 2008). Furthermore, the production of bio-based raw materials (such as corn, sugar cane, or soy for feedstock) may or may not be associated with lesser greenhouse gas emissions and consumptions of fossil resources, but may have *equal or greater impacts* in other impact categories (e.g. land use, toxicity related to using pesticides, eutrophication related to using fertilisers) than fossil-based materials (see Chap. 30 for further details). These phenomena are commonly referred to as burden shifting (e.g. between environmental issues or compartments). Identifying these is a fundamental application principle unique to LCA.

LCA is a tool that can be useful for comparing products and processes for identifying such burden shifting and how to minimise impacts across a variety of impact categories. However, it is important always to ensure as a practitioner that all relevant chemical emissions are inventoried and all impact pathways are characterised. These general cautions are also relevant for LCA studies focusing on chemical synthesis and production processes as discussed in the following section.

31.2.2 Chemical Synthesis and Production Processes

LCA is a useful tool for improving existing processes and designing new processes for the synthesis and production (Fig. 31.3, stages A–D) as well as for the end-of-life treatment (Fig. 31.3, stage F) of chemicals and chemical products, to inform process systems engineering decisions (Jacquemin et al. 2012). In this section, LCA case studies focusing on chemical synthesis and production processes across various economic sectors are discussed.

A major issue illustrated by several LCA studies is that management decisions based on single indicators or criteria can lead to increasing other impacts (that were not considered in the decisions), thereby indicating the strength of LCA as an approach to assess multiple indicators and related trade-offs. An example is the development and application of new plant protection products (pesticides) designed with the intention to reduce human toxicity and ecotoxicity potentials associated with emissions after application in agricultural crop protection or elsewhere (e.g. household pesticides). A related LCA study revealed that the production of a new and more effective plant growth regulating pesticide with less intrinsic toxicity (preferable from a risk perspective) than a functionally equivalent earlier marketed pesticide comes at the expense of increased impacts associated with pesticide synthesis and production processes (Geisler et al. 2005). The higher impacts for the new pesticide are mostly explained by the high complexity of its molecular structure requiring more synthesis and processing steps. In general, impacts related to the production of chemicals have been attributed to energy consumption which tends to increase with increasing complexity of a chemical molecule. Highly specialised chemicals, such as pharmaceuticals, can thereby be associated with higher energy consumption and related impacts from synthesis and production processes than other chemicals (Wernet et al. 2010).

Not only complexity of chemical synthesis and production processes, but also the difference in raw materials used drives environmental performance profiles of chemicals and chemical products. This is shown in another set of LCA studies contrasting chemical production from fossil fuel-based versus renewable (bio-based) resources. Synthesising and producing chemicals from biomass (e.g. sugar cane) instead of from fossil fuels (e.g. petroleum or natural gas) has been proposed as a 'sustainable technology' with respect to reducing reliance on fossil resources and greenhouse gas emissions. However, a full sustainability analysis has typically not been conducted, which is why several LCA studies have focused on this claim.

As an example, a simplified overview of the different chemical synthesis and processing steps involved in polyethylene terephthalate (PET) polymer production is given in Fig. 31.5. While terephthalic acid used in the production of the chemically identical PET and bio-PET is in both cases derived from petroleum, ethylene glycol can be derived from natural gas as a fossil resource (for PET) or from sugar cane as a biomass feedstock (for bio-PET). The process of natural gas refinement to create ethylene glycol alone consists of several steps including cracking (breaking down) into ethylene and other chemicals, ethylene separation and purification involving several distillation processes (not shown in Fig. 31.5). Accordingly, LCA studies have found that bio-based chemical production usually can lead to less greenhouse gas emissions than fossil-based chemical production, mainly because less refinement of fossil fuels is required. However, growing, harvesting and processing bio-based feedstocks may lead to other impacts related to agriculture production systems, e.g. land use (see Chaps. 29 and 30), which are highly variable with respect to the type of biomass used (Tabone et al. 2010; Akanuma et al. 2014). Furthermore, the type of biomass used can influence the energy required, and

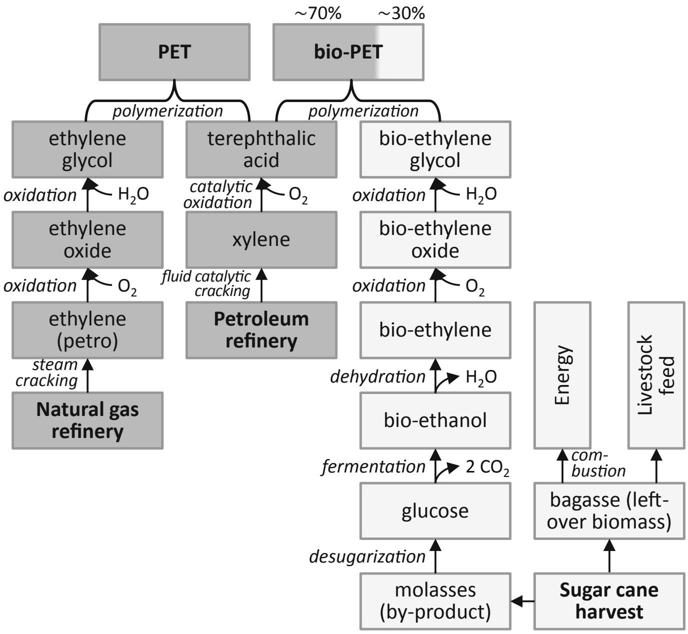

Fig. 31.5 Production process steps for chemical synthesis of polyethylene terephthalate (PET) derived from fossil fuels and bio-PET (partly) derived from bio-resources (modified from Tabone et al. 2010)

post-processing of bio-based products and residues greatly influence the overall related environmental performance.

Other LCA studies have focused on specific aspects of chemical synthesis and processing, such as comparing continuous and batch reactor types (e.g. Wang et al. 2013) or different catalysis and fermentation processes (e.g. Pati et al. 2014). It is further important to consider which catalysts are used in other processing steps that petro- and bio-based materials like PET have in common, such as antimony trioxide found at concentrations of 200–300 ppm in PET or other, metal-free catalysts used in the polycondensation process as part of polymerisation. Several studies have concluded that processes with higher yields have a lower impact per chemical production unit. The use of solvents has additionally been identified as an important component influencing environmental performance of chemical products (De Soete et al. 2014). Generally and specifically for chemical synthesis and processing it is important to be sceptical of processes and products labelled or deemed ‘green’ or ‘sustainable’ without performing a full LCA as shown, e.g. for ‘green’ nano-materials synthesis (Pati et al. 2014). An overview of aspects that are relevant for assessing ‘green’ chemical synthesis and production processes is given by Kralisch et al. (2015).

31.3 Specific and General Methodological Issues for LCA of Chemicals

Applying LCA, specifically in the chemical and pharmaceutical sectors, and in other sectors where chemicals play a central role, comes with several methodological and practical challenges. Generally, gathering chemical inventory data, quantifying impacts, and interpreting results constitute challenges for LCA studies across sectors. In the following sections, some of the most relevant challenges focusing on chemicals in LCA are discussed in relation to the definition of the goal and scope of an LCA study, product system modelling and quantification of life cycle chemical emissions in the inventory analysis, characterisation modelling in the impact assessment, and finally interpretation of LCA results in different contexts.

31.3.1 Goal and Scope Definition

Consistently defining the goal and scope for chemical products or processes (e.g. functional unit of the considered product or service system and related reference flow(s) and system boundaries) is not trivial and needs to be critically considered by a practitioner. Examples of relevant issues when defining functional unit, reference flow(s), and system boundaries are discussed in the following.

Functional Unit (FU)

LCA (and other types of assessments) can be designed to compare functionally equivalent chemicals and chemical products as classified by *chemical function* (e.g. solvents, catalysts), *material function* (e.g. nanotubes, polymers) or *product function* (e.g. herbicides). It is hence important to define the level of 'functionality' based on which a study will be conducted. This functionality must be captured in the definition of the FU of an LCA study as basis for comparing products or systems.

Performing an LCA study is useful for providing valuable insight into which of two alternative, functionally equivalent chemicals or products provides the function with the lowest overall environmental impact profile, thereby focusing on avoiding burden shifting between different types of environmental impacts. To screen multiple alternatives to harmful chemicals in a particular product application, in contrast, the focus often is not mainly on environmental performance, but on a combination of regulatory compliance, economic and technical feasibility, along with considering hazard and human, environmental and social impacts. In such cases, a chemical alternatives assessment (CAA) might be the preferred approach to identify the most viable solution(s).

Chemicals and chemical products can also fulfil more than a single function and, hence, a partial definition of the functional unit could lead to inconsistent comparisons if the appropriate product systems are not considered as demonstrated in Example 31.1.

Example 31.1 **Functional Unit (FU)** Take a cosmetic product like shampoo, where different chemical ingredients provide different functions as part of the final shampoo product, e.g. to provide clean, shiny and fragrant hair for one person over 24 h. If the **FU is defined** with respect to a single shampoo product (one-product system) that **cleans the hair of one person** (by containing detergents) **and makes it shiny** (by containing siloxanes) **for 24 h**, a functionally equivalent service could be also provided by applying two distinct products (two-product system), one being a shampoo that only cleans hair (and does not make it shiny) and another being a conditioner that makes the hair shiny (and does not clean). However, both the one-product and two-product systems should not provide fragrance in order to be consistently compared via the same FU (underlined text above) that excludes fragrance.

Likewise, if the FU is defined to just clean hair for one person over 24 h, comparing LCA results of a shampoo that only provides clean hair to a shampoo that provides clean, shiny and fragrant hair could yield the misleading outcome that the former shampoo 'performs better', because the production and related impacts of additional chemicals of the latter shampoo (containing siloxanes for making the hair shiny and terpenes for making the hair fragrant) are related to functions not fulfilled by the shampoo that only cleans hair. Hence, the comparison would be biased by comparing products fulfilling distinct functions.

Defining an appropriate FU for multi-functionality (see Chap. 8) is also important. For example, water and propylene glycol are both effective chemical solvents and, thus, both would fulfil an FU defined with respect to providing the function of a solvent in, e.g. a shampoo product. Propylene glycol, however, provides other functions that water does not provide (e.g. stabiliser, humectant, emulsifier). Therefore, a comparison of propylene glycol and water in an LCA study based on a solvent-based FU would not capture the multi-functionality of propylene glycol. Defining the FU with respect to all functionalities and then providing system expansion when necessary (e.g. water plus a stabiliser plus a humectant plus an emulsifier is functionally equivalent to propylene glycol in shampoo) can be an important consideration in any LCA on chemicals or product systems. It is, hence, important to ensure the product(s) or chemical(s) investigated in an LCA study are functionally equivalent and the FU captures this equivalency appropriately.

Reference Flow

The reference flows (Chap. 8) in an LCA study reflect the overall amount of goods and/or services that are required to fulfil the defined FU. Taking a no-wash (dry) shampoo versus a conventional (liquid) shampoo as examples, the reference flows to fulfil an FU of cleaning the hair of one person for one day could be 10 g of the liquid shampoo product plus the (hot) water used to wash the hair. The reference flow for the dry, leave-in, no-wash shampoo could be simply 5 g of powdered product (with no wash-water needed). Furthermore, if functionally equivalent products or chemicals provide different efficiencies to fulfil a defined FU, the different efficiencies need to be accounted for in the reference flow. This issue also points to a problem for cradle to gate LCA studies on chemicals, where it is possible that a chemical could have greater cradle to gate impacts than another chemical per unit mass emitted, but far less of the former chemical is required to fulfil the same FU. Here, pesticides with different efficiencies towards the same pest offer a typical example.

System Boundaries

The system boundaries (Chap. 8) of any defined chemical product or service systems in an LCA study need to capture all relevant processes for the systems being compared. For example, if the purpose of an LCA study is to compare bio- with fossil-based chemical synthesis, the system boundaries must include and differentiate all raw material acquisition processes, namely all refining processes for the fossil-based chemical and the crop production and processing steps for the bio-based chemical (see also Fig. 31.5). However, for these systems, it may not be relevant to include chemical use and disposal stages in the study, whenever these life cycle stages are equivalent in both cases. Such systems are referred to as 'cradle to (factory) gate' systems and are common in LCA studies on chemical synthesis and other chemical production processes (Jimenez-Gonzalez and Overcash 2014). In contrast, if the purpose of the study is to compare two distinct fossil-based materials fulfilling the same function, the disposal stage could be a relevant driver of the difference between the compared product systems.

For several chemical products and production processes, consistently defining system boundaries is challenging. An example is the application of plant protection products containing chemical pesticide active ingredients (e.g. carbamate insecticides) applied in agricultural crop production, where the FU could be defined to provide a specified amount of crop in a season. Allocating field buffer strips (i.e. non-agricultural areas that are among other functions introduced to reduce the impact of applied pesticides on non-treated areas), which may be required by law, to the technosphere would apparently influence the crop yield per hectare and amount of pesticide used compared with an equivalent system, where the buffer strips are defined as part of the environment (Rosenbaum et al. 2015). Including buffer strips in the considered technosphere system or not will, hence, influence the related impacts and also defines the scope of the environmental distribution processes of pesticides in the LCI and LCIA phases. As a consequence, the definition of the system boundaries needs to be aligned with the selected pesticide inventory data and characterisation models to avoid overlaps, double counting of processes and potential gaps along the pesticide impact pathways.

31.3.2 Product System Modelling and Inventory Analysis

There are several obstacles that need to be considered in the product system modelling and inventory analysis phase (Chap. 9), after the goal and scope of an LCA study have been defined.

Data Availability and Quality

All relevant chemical elementary flows from a given product system to the environment need to be quantified in the LCI phase. When using LCA software, emission quantities are often available through an LCI database, for example for processes occurring in Europe or the 'rest of the world.' LCI databases generally rely on typical or average emission inventories or an inventory taken by one industry for a given unit process, which may be outdated or tied to, e.g. a specified electricity mix. Thus, it is always preferred to gather primary data, especially for the foreground system modelling (Chap. 9), of the specific LCA case under study. This poses a particular challenge to LCA practitioners, who may or may not have access to company-specific data to resolve the nuances of a particular supply chain. While in some cases, a particular commissioner of an LCA study might provide such data, while in other cases such data have to be collected from different parties. An example is the application of plant protection products, where pesticide manufacturers will know the concentration of a pesticide active ingredient in a formulation product, but where the different farmers might know the effectively used amount that is applied on agricultural fields and this usually depends on pest-, climate-, soil- and application-specific conditions.

Emission Estimation and Modelling

Most chemical synthesis and material/product manufacturing processes involve several steps, which can yield usable by-products that have to be considered in an LCA study (see Chap. 9 for further details). As an example, harvesting sugar cane yields refined sugar, but also molasses (sugar refining by-product) and bagasse (dry leftover biomass after extracting the juice from the sugar cane). While molasses can be further used to produce biochemicals, bagasse is usually burned (for energy conversion) or used as livestock feed (Fig. 31.5). In an LCA study, usually only one of these products (sugar, biochemical, energy, livestock feed) is in focus and the other products must be accounted for through subdivision or system expansion or if it cannot be avoided through different types of allocation (see Chap. 9).

When building a product system model, different tools and software packages are available. Specifically for simulating material and energy balances of chemical production and processing, there exist several (open-source and commercial) chemical process simulators, such as Aspen HYSYS for oil and gas process simulation and Aspen Plus for chemical process optimisation (www.aspentech.com), BatchReactor and BatchColumn for chemical reactor and batch distillation columns simulation, respectively (www.prosim.net), or CHEMCAD software suite for chemical process simulation and optimisation including batch operations (www.chemstations.com). Such software packages may include proprietary data from the chemical and other industries that are otherwise not accessible and may intrinsically use different allocation systems. The responsibility of ensuring transparency and consistency when building a product system including proper consideration of co-products and by-products lies with the LCA practitioner. However, several documents exist for LCA practitioners to seek guidance, and working examples of co-product consideration for the chemical industry can be found elsewhere (e.g. Weidema 2000; Karka et al. 2015).

In most LCA studies, an inventory covers hundreds of processes and emission flows but not all chemical emissions are usually able to be covered. Often missing from LCI databases are, e.g. emissions to the occupational and consumer environments, and the ingredients (e.g. chemicals) in a product, which can be emitted indoors during product use or outdoors post-use as demonstrated in Example 31.2.

> ***Example 31.2*** **LCI Emission Pathways** When a **consumer product** (e.g. perfume) or industrial product (e.g. agricultural pesticide) is used, the chemicals within the product undergo various pathways, thereby exposing for example the product users and people nearby. Consider that a colleague at work **applies an air freshener or perfume in the office**. Perhaps you smell or even taste it in the first minutes after application (indication of exposure), maybe the scent remains in the office for some days (indicating sorption and desorption from indoor walls and other surfaces), and maybe you can even smell it just outside the office building (indicating transport outdoors via ventilation).

In some cases, a large proportion of chemicals within products can be taken in by humans during and after product use, which is a major concern amongst regulators and researchers. In LCA, such considerations are currently largely missing, but first efforts were made to include indoor fate and exposure pathways (referred to as 'near-field') into the toxicity characterisation model USEtox 2.0 (http://usetox.org). Without accounting for near-field fate and exposure pathways, LCA studies typically may assume a fixed-fraction like 100% of product ingredients being emitted to the environment. In general, assuming such emission distributions could lead to an underestimation of resulting human toxicity potentials and an overestimation of environmental or ecosystem impacts. This is illustrated in Fig. 31.6 for d-limonene as commonly found chemical in a shampoo product, where assuming 100% of the used product being washed-off (left-side pathway in figure) instead of modelling a more complex yet more realistic distribution (right-side pathway in figure) yields a difference of more than three orders of magnitude for freshwater ecotoxicity impacts, which is significantly beyond the uncertainty range for this impact category.

Emissions can also occur from chemical residues in products that are related to cross-contamination, i.e. such chemicals are not purposefully added to a product and enter a product from using, e.g. recycled material where not all chemical ingredients are known. Often, inventory data related to cross-contamination

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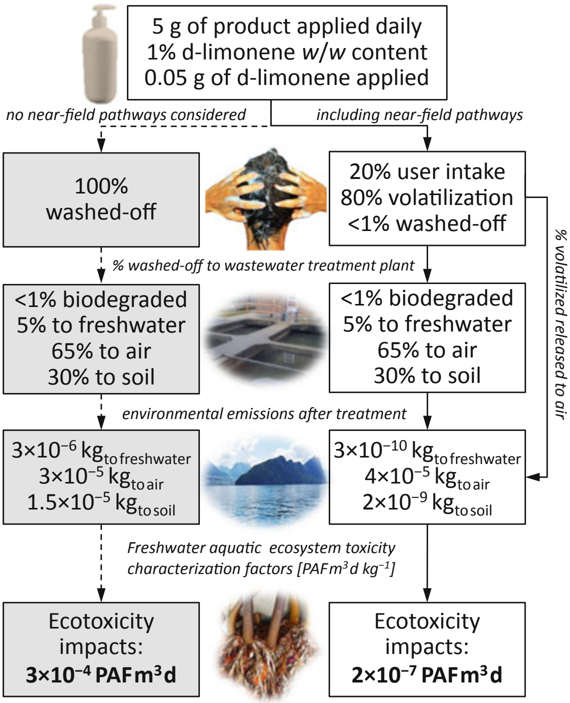

Fig. 31.6 Illustrative example of assumptions for emission distributions of chemicals in consumer products in life cycle assessment showing a substantial decrease in the estimated potentially affected fraction (PAF) of freshwater species from the chemical ingredient d-limonene (CAS: 5989-27-5) in shampoo when accounting for indoor fate and exposure of cosmetic products. Adapted from results from Ernstoff et al. (2016a) combined with freshwater ecotoxicity characterisation factors from USEtox 2.0 (http://usetox.org). Air emissions were assumed to be to urban air, water emissions to continental freshwater, and soil emissions to continental natural soil

pathways are very limited if at all available. Using similar processes or pathways as proxy might be a possibility to address this limitation, but also introduces additional uncertainty in the emission estimates.

Spatiotemporal Variability in Emissions

Time (e.g. year, season or duration) and location can influence variations in emissions, referred to as 'spatiotemporal' variability. In many cases, LCI results do not capture the time of emissions from systems, e.g. agricultural practices (e.g. harvesting, applying fertilisers) can occur according to daily or seasonal cycles according to the geographic location of the farm. Likewise, emissions of landfill leachate are influenced by changes in environmental conditions (e.g. acidity and temperature) which can change through time and according to location (Bakas et al. 2015).

Incomplete Emission Inventories

It is important to be aware of the incompleteness of some emission inventories. For example, energy conversion processes generally are well detailed in LCI which can result in high toxicity related impacts resulting from energy consumption, but other processes, e.g. related to chemical processes may have less complete inventory and, hence, related toxicity impacts might be underestimated (Laurent et al. 2012).

31.3.3 Impact Assessment

Characterising chemical emission flows resulting from the LCI in terms of their impacts on humans and the environment requires a careful consideration of study context (e.g. spatial region), number and relevance of chemicals to be characterised (in many cases, most chemicals contribute marginally to overall impacts, while only few chemicals dominate overall impact profiles). In the following, challenges and pitfalls in the impact assessment of chemical products and processes are discussed with focus on toxicity-related impacts, where special challenges exist mainly due to the countless chemicals to be characterised and the complexity of related impact pathways.

Limited Substance Coverage

USEtox, a scientific consensus model for characterising human and ecotoxicological impacts of chemicals, presently provides characterisation factors for more than 3000 chemicals, which constitutes the largest list currently available in LCIA (http://usetox.org). However, with tens of thousands of chemicals on the market, inventoried chemical emissions either documented in an LCI database or by a practitioner investigating a specific system or process, may in many cases not have existing characterisation factors or the data required to develop new characterisation factors (e.g. toxicity dose-response information). This limitation to substance coverage in LCIA is important when interpreting results, because a lack of data for many chemicals does not preclude their possible impacts.

Chemical Degradation Products

When a chemical does not degrade, or degrades very slowly, it is considered ‘persistent.’ Persistent chemicals thereby can be linked to greater impacts because they are not or very slowly removed from the system through degradation. In current LCIA methodologies, abiotic (e.g. where a chemical is transformed via interactions with sunlight) and biotic (e.g. when a chemical is metabolised by soil bacteria) degradation essentially ‘removes’ organic chemicals from the system and no further impacts are characterised. In reality, degradation processes transform a chemical into various degradation or transformation ‘products’, including other chemicals or gases, which can also impact the environment. Degradation products can have greater or lesser impacts than their parent compounds, for example aminomethylphosphonic acid (AMPA), which is the main degradation product of the broad-spectrum herbicide glyphosate, is more persistent and more toxic than the glyphosate parent compound. As an example, not considering AMPA in an LCA study that considers agricultural processes where this herbicide is used could underestimate the impacts of using glyphosate. Therefore, an LCA practitioner should include estimates of persistent degradation products and appropriate characterisation factors (in this case for AMPA, not glyphosate) to better capture the impacts of chemicals. While this approach will not be feasible for all chemicals (due to data limitations), it should be performed when the issue is known and data are available.

Impacts from Chemical Mixtures

Impacts towards humans or different ecosystems, related to chemical emissions, are a function of the simultaneous prevalence of other chemicals, which might have synergistic (enhancing) or antagonistic (counteracting) properties with respect to the effect of a considered chemical. Since information on the site-specific mixture of chemicals in any environmental medium or compartment is not usually available, and the impacts of such a mixture on humans or the environment are not known, synergistic or antagonistic effects are usually not considered, and instead additivity of concentrations and effects is assumed. This means that the effects of all chemicals contributing to the same impact category, e.g. freshwater aquatic ecosystem toxicity or ozone depletion, are summed up to arrive at an overall product system-related impact score. If for any LCA study the emission location and time is known and related background concentration profiles available for all relevant chemicals, this assumption could be evaluated by identifying and quantifying the synergistic or antagonistic effect potentials. However, the potentially added accuracy in an LCA context is most likely not relevant given existing uncertainty attributable to other aspects in the characterisation of chemical emissions. Besides, the large number of chemicals present and emitted into the environment yields an almost limitless amount of possible mixtures, rendering it impossible to quantify the specific effect potentials for each mixture.

Missing Fate and Exposure Processes and Pathways

In order to reduce the demand put on LCA practitioners, streamline workflows, and allow for science-based and consensus-driven solutions, LCIA often relies on predefined methodologies. However, hundreds or even thousands of chemicals might be inventoried for various processes in an LCA study, but characterisation factors or a LCIA method for a given impact at mid-point or end-point level may be missing, especially for toxicity-related impacts (see Chap. 10). Moreover, certain exposure settings (occupational, consumer) or routes (e.g. dermal exposure) or target organisms (e.g. exposures of bees) may be missing from an LCIA model. Effect factors may also be missing or inconsistent, e.g. in the case of human toxicity, effects of allergy or endocrine disruption (i.e. interaction with the hormone system) are often not included, but may be highly relevant for chemicals in consumer products. Finally, many of the methodological gaps in LCIA are also due to the reliance on simplifying assumptions. The LCA practitioner, who is constrained by resources (time, money, data access), is responsible for compiling the necessary data and for ensuring that the LCIA methodology chosen (or developed) is suitable for the defined goal and scope of an LCA study. Specifically, to characterise a chemical's impact, several assessment factors are required and must be sufficiently scrutinised within the chosen LCIA method, such as the chemical environmental fate, ecosystem and/or human exposure if relevant, and subsequent effects with respect to given impact categories. Each of the related data requirements poses its own challenges. To avoid the misleading conclusion that missing aspects of the chosen LCIA method do not cause impacts because they were not assessed, it is important to be familiar with which processes (e.g. biotransformation), environmental compartments (e.g. indoor air), exposure pathways (e.g. dermal uptake), and effects (e.g. endocrine disruption), may be missing from the selected characterisation methods but are relevant for the system under study. In some cases such missing aspects can be addressed by the practitioner by developing new methods or by adapting existing methods; if not, it is important to be aware of how this could influence results.

Spatiotemporal Variability of Impacts

LCIA methods are generally based on regional or global averages for various chemical, environmental and pathway data and processes, e.g. how long it takes chemicals emitted to freshwater to reach the sea (i.e. residence time), or how many persons live in an urban area (i.e. population density). Studies have shown, intuitively, using a continental average instead of 'spatially differentiated' regionalised models can yield large uncertainty in the estimated impacts (e.g. Kounina et al. 2014). Thus, if the location of the emissions (e.g. from a specific factory) in an LCA study is known, using a model with characterisation factors specific for that region can reduce uncertainty of model results. If emission locations are not known (as is the case for most chemicals in typical LCA studies), characterisation results for regions can be applied that are parameterised, i.e. averaged for the characteristics of a particular region. The same rule applies for temporal aspects, where in LCA mostly steady-state conditions and continuous emissions are assumed, which might not be true for, e.g. agricultural pesticides that are applied on specific days only (i.e. pulse emissions). In such cases, accounting for the dynamics of the chemicals in the modelled environmental system may reduce uncertainty in characterisation results (e.g. Fantke et al. 2012), but whenever temporal information on emission patterns is not available, parameterised characterisation results can be applied that account for the most important temporal aspects of a modelled system.

Impacts Versus Benefits

Life cycle *impact* assessment inherently focuses on quantifying 'negative' impacts on humans and the environment. A stakeholder could in some cases argue that their product or service offers a benefit to society that is not accounted for, meaning that LCA yields misleading results. When facing such an argument as LCA practitioner, it is important to go back to the fundamentals of LCA. The impact assessment phase of LCA is designed to assess environmental 'benefits' in the form of 'avoiding environmental impacts.' For example, a wastewater treatment plant design that also decreases environmental pollution compared to another design offers a 'benefit' that is quantifiable in an LCA context (see Chap. 34 on LCA of wastewater treatment). Furthermore, when comparing functionally equivalent products or services, their benefits (e.g. restoring a wetland to yield a level of biodiversity, or designing a car with a certain safety rating) is often captured in the functional unit of an LCA study, which defines a unit of the (beneficial) service being provided. There are special cases where considering societal benefits that are not captured in the functional unit or by the assessment methods can be extremely important when guiding decision-making. In some cases, LCA may not be the appropriate tool to assess such benefits; however, developing LCA-compatible methods to quantify societal benefits (specifically positive human health outcomes) is a topic of high interest when assessing human nutrition and dietary patterns, where two functionally equivalent diets can have very different health impacts (Nemecek et al. 2016).

31.3.4 Interpretation

The interpretation of results is fundamental for the findings and reliability of every LCA study and subsequent guidance provided to stakeholders, and to LCA in general (see Chap. 12). Robust and transparent interpretation of results from an LCA study can offer sound council for the stakeholders and when aggregating with other LCA studies can elucidate generalisable findings important for sustainable development. As an example of nuances of interpretation, the 'New Plastics Economy' report (WEF 2016) cites interpretation of several LCA studies and implies that a major shortcoming of LCA is its inability to identify and support 'target states', such as moving towards increased production and use of bio-based plastics. Indeed, as previously discussed, LCA studies on bio-based versus fossil-based plastics have demonstrated similar, if not greater impacts (e.g. on land use and toxicity potentials) for bio-based plastics due to agricultural practices (see Chap. 30), which is a finding that may be unintuitive or undesirable to some (e.g. stakeholders in the bioplastics industry). When interpreting such LCA results, it is important to distinguish what an LCA says about 'here and now' versus what it could mean for future sustainability goals or targets of stakeholders. For example, LCA results showing bio-based plastics have 'greater impacts' than fossil-based plastics do not discredit bio-based plastics as a sustainability *goal*, but they do indicate that bio-based plastics face sustainability challenges given current agricultural practices, which thus must be addressed to avoid impact trade-offs. Furthermore, LCA results can help indicate which feedstock is the most eco-efficient (less impacts per kilogram) to work towards a bio-based 'target'. In practice, LCA may not be able to easily identify target states often elucidated according to societal values (which may include socioeconomic or political factors) or intuitive/consensual sustainability goals, but LCA can be instrumental in reaching goals and target states in a holistically sustainable manner and shedding light on challenges faced when working towards such goals. In the following, some additional challenges in interpreting LCA results are outlined.

Contribution to Impact Results

Especially for LCAs on chemical products or processes, it is important to transparently report and document the contribution of different chemicals to impacts related to product life cycle stages and individual processes. This can help identify potential problems in the processing of LCI or LCIA results (e.g. if one chemical dominates results). Interpreting LCA results might be particularly challenging if it is not clear whether toxicity-related impacts are associated with chemical *emissions* occurring along the product life cycle or, in contrast, with chemicals that are product *ingredients* (Roos and Peters 2015). As an example, glass used as food packaging can show higher potential toxicity impacts compared with plastic packaging due to transport-related emissions of toxic chemicals from fossil fuel burning (Humbert et al. 2009), which is linked to the fact that glass is usually heavier than plastic. However, plastic food packaging can likely lead to greater exposures to various chemicals through food than glass, but this aspect is not (yet) considered in current LCIA toxicity models (Ernstoff et al. 2016b). Further, it might be unclear whether worker and/or consumer exposure pathways are included as these are currently beyond the scope of LCA studies focusing primarily on environmental emissions. The covered pathways and exposed populations should always be clarified in an LCA study to avoid possible misinterpretation of results. This is of specific relevance for the comparison of chemicals and chemical products and processes, where such ambiguities can cause confusion regarding the contribution of chemicals and related impact pathways and life cycle stages are lacking.

Identification of Considered Chemicals

In any of the aforementioned contexts, it must be acknowledged that most chemicals have various common names (lindane, CAS RN: 58-89-9, is for example also commonly known as HCH, hexachlorobenzene, or cyclohexane, etc.). Hence, it is important to ensure that names for chemicals in the different phases of an LCA study (e.g. inventory analysis and impact assessment) are consistently chosen based on using CAS registry numbers or similar as chemical identifier to, e.g. avoid double counting or neglecting chemicals with ambiguous names. This exercise can prove to be challenging as LCA software packages often report chemical inventories by chemical name and not by CAS number.

Quality and Uncertainty

Quality checks across the large number of inventoried chemicals is usually difficult, but inventory results should nevertheless be verified by, e.g. checking the mass balance of only those chemicals that drive overall impact results, for examples heavy metals that dominate toxicity impact profiles. Furthermore, it is essential to report and discuss uncertainties of LCA data and results with respect to each impact category as integral part of the analysis, and consider such uncertainties in the interpretation of results and guidance provided to decision makers (see Chap. 11).

Particularly uncertainty associated with toxicity characterisation results is high compared with other impact categories and results can furthermore differ between toxicity characterisation methods, which can in some cases influence the overall ranking of compared product systems. Uncertainty (lack of data or understanding) and variability (data heterogeneity) are distinct concepts, but are sometimes (incorrectly) aggregated. For example, often 'high uncertainty' is perceived negatively or seen to discredit a particular LCIA method. However, such 'uncertainty' can be a direct reflection of reality and variabilities in temporal and spatial chemical fate and organism disease responses (see Chap. 11 for further details). Likewise, if an impact category has low or no associated uncertainty, this is perceived as positive but should in fact be a warning sign that there may be a lack of understanding of what uncertainties and/or variabilities exist or that the environmental relevance (or representativeness) of an indicator may be low (which introduces an uncertainty in the interpretation phase, but this is usually not quantified). To begin transparently addressing this issue, impacts should ideally be cross-compared using different LCIA characterisation methods with particular focus on identifying which chemicals contribute the most to impacts in each LCIA method (which are often not the same). Moreover, uncertainty ranges for toxicity-related impacts should be reported in logarithmic scale to put average uncertainties of two to three orders of magnitude into perspective of more than 15 orders of magnitude in the variability across chemicals. This is shown in Fig. 31.7 for 786 chemicals with available measured ecotoxicity effective concentrations for 50% of the exposed species (EC50; mg/L) for aquatic ecosystems. EC50 values are used to calculate effect factors as part of toxicity characterisation in LCIA (see Sect. 10.11). The relation between uncertainty and cross-chemical variability is not much different for toxicity impacts than for other impacts, where uncertainty in characterisation results (of usually only a handful of contributing chemicals) and related variability across contributing chemicals are both less broad. However, uncertainty ranges vary widely between chemicals, but chemical-specific uncertainty around characterisation factors is usually not available in LCA, except for specific pathways, e.g. exposure to pesticide residues in food crops (Fantke and Jolliet 2016), where also the underlying method to quantify chemical-specific uncertainty is outlined.

Comparison with Results from Other Methods

Comparing results from an LCA study with results from a different method can help identify methodological inconsistencies that require further inspection. As an example, it might be desired to compare the ranking of chemicals in terms of their potential toxicity impacts on humans and/or ecosystems in an LCA study with the ranking of chemicals based on persistence, bioaccumulation and toxicity or other criteria used, e.g. by risk regulators. In this context, it is important to acknowledge that inconsistencies can result from the primary data used in an LCA versus another

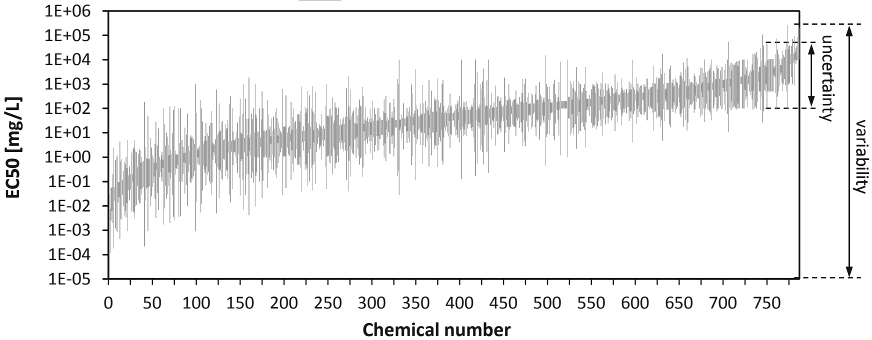

Fig. 31.7 Ranges of measured chemical-specific ecotoxicity effective concentrations (50% of exposed species affected), EC50, for aquatic ecosystems collected and indicated as reliable for 786 chemicals based on REACH (echa.europa.eu/regulations/reach)

method, or assumptions and cut-offs may be based on different criteria, e.g. worst case versus best estimate or most sensitive species versus average ecosystem sensitivity (Harder et al. 2015). This might lead to problems when comparing chemical rankings based on different assessment methods and data sources. Chemical toxicity results may furthermore differ between regions, countries or assessment methods, and thereby the consideration of chemicals as, e.g. 'non-carcinogenic' in LCA toxicity characterisation models may not be consistent with a specific regulatory context, such as the Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) legislation framework of the European Union.

31.4 Conclusions

Stakeholders commissioning an LCA study can drive the goal and scope, the selection of inventory processes, and the selection of impact categories. In many cases, this can lead to an assessment that is restricted, for example to greenhouse gas emissions and a focus on climate change. The limited scope of such studies must be considered in the interpretation and application of their results, whenever other important impact pathways for chemical production, use, and disposal are not assessed. It is always important to be critical towards LCA outcomes and understand their limitations and scope, and respect that no tool (including LCA) can answer all questions related to chemicals and sustainability.

Not only can the scope of an LCA study be intentionally restricted according to its goal and scope, but there are several remaining challenges that also limit LCA, such as partial coverage of chemical inventory data, fate modelling (e.g. regional variation), exposure pathways (e.g. dermal exposure of consumers), and characterisation of potential human and ecosystem toxicity impacts. Given that there are tens of thousands of commercially used chemicals, and often little data on their properties or effects, the challenge of addressing chemical risks and impacts is not unique to LCA. Generally, the various methods for characterising risk and impacts of chemicals face similar challenges of data availability, but they also face methodological challenges and intentional differences. For example, results of an LCA addressing several impact categories and hundreds of chemicals, where often the exact emission location and timing is unknown, are difficult to cross-compare with results of a toxicity-focused risk assessment considering specific (e.g. worst-case) conditions and only one or several chemicals of concern (Harder et al. 2015).

Attempts of combining LCA with principles of green and sustainable chemistry, integrating LCA- and risk-based approaches, and including life cycle impacts in chemical alternatives assessment frameworks demonstrate the growing complementarity and relevance of the life cycle approach in other science-policy fields (Jimenez-Gonzalez and Overcash 2014; Harder et al. 2015; Jacobs et al. 2016). Overall, the number of LCA studies focusing on chemicals or chemical products or processes is growing; thus, increasing discourse and trust in LCA methods as well as improving existing inventory and impact characterisation approaches.

Over the past years of research, LCA has developed into a powerful tool to identify and assess trade-offs and burden shifting between different environmental issues, identify hotspots and minimise overall environmental impacts of chemicals in the life cycle of products and processes. With rising interest in creating 'environmentally friendly' chemicals and products, LCA is particularly important to help avoiding 'green washing' and unsupported claims. A common example is the comparison of products that can be developed purely from petrochemicals and also from a combination of petro- and biochemicals. Larger potential greenhouse gas emissions in the petrochemical production are confronted with often larger land use and pesticide-related toxicity impacts from agricultural crop production when serving as feedstock for biochemical production (Tabone et al. 2010; Cespi et al. 2015). Only comparing climate change impacts in this context would lead to false conclusions (i.e. that bio-based chemicals are always 'greener') and does not help identify how to optimise production processes and resource use when moving from petrochemicals to biochemicals in, e.g. plastics production. This is especially relevant when assessing emerging technologies, where there is a high level of optimisation potential in the years to come for upscaling lab-level processes to a commercial level.

Future research related to chemicals and LCA should focus on identifying and resolving areas of high uncertainty (such as changes through space and time), filling data gaps (for example with high-throughput exposure and toxicity modelling approaches), and addressing issues of high concern such as consumer and occupational exposure and other toxicity endpoints (e.g. toxicity to bees). Furthermore, applying LCA in case studies and analyses to address issues of existing and emerging technologies can help pinpoint and corroborate solutions towards more sustainable production and consumption of synthetic and naturally occurring chemicals. AQ1

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