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The role of Life Cycle Assessment in Safe and Sustainable by Design: Lessons learned from a case study on plasticizers

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Abstract

Safe and Sustainable by Design (SSbD) is a concept introduced in the Chemical Strategy for Sustainability of the European Commission, with the ambition of guiding innovation in chemicals and materials design toward the minimization of impacts on human health and the environment. To operationalize this concept, the European Commission Joint Research Centre developed a scientific framework, which integrates safety and environmental sustainability considerations. Such a framework was then adopted by the European Commission as a recommendation, for the use of companies and research institutes working on the development of chemicals and materials. The framework brings together two different aspects: safety and environmental sustainability. Safety is addressed looking at intrinsic properties of the chemicals and assessing risks related to exposure scenarios for workers, consumers, and environment, while the environmental sustainability aspect is assessed via the application of Life Cycle Assessment (LCA) following the provisions of the Product Environmental Footprint method. The goal of this study is to test via a case study the use of LCA to assess six plasticizers, assessing the framework's applicability and proposing approaches to address challenges and research needs. Indeed, while literature on LCA of chemicals is expanding, there are still a number of open issues to be addressed. Seven pivotal challenges are presented and discussed in this study. They cover all the phases of the life cycle, from the goal and scope (benchmark definition and application to intermediate products) to Life Cycle Inventory (LCI) (availability of data, modeling of end of life, additional information and innovation perspective) and Life Cycle Impact Assessment (LCIA) (e.g., comprehensively addressing impacts related to substances of concern). The case study examined and the seven identified challenges are starting points for improving the implementation of the Safe and Sustainable by Design framework, promoting sustainable innovation in the manufacturing of chemicals and materials.

Keywords: Safe and Sustainable by Design, Life Cycle Assessment, substitution, plasticizers

Introduction

The manufacturing and use of chemicals and materials plays a paramount role in global CO_2 emissions and as a driver of different environmental impacts. In 2022, among the industrial sectors, the production of chemicals from fossil fuels, cement, and steel were the top three both in energy consumption and direct CO_2 emissions, according to the International Energy Agency (IEA, 2018, 2025). Moreover, there is solid and growing evidence of environmental and human health effects due to chemical exposure. As an example, a study of the European Commission (EC, 2017) reports that exposure to endocrine disruptors alone cost 157 billion euros in health care and lost earnings. The global demand for chemicals is expected to grow by almost 30% by 2030, accounting for over 95% of the increase in oil demand (IEA, 2018, 2023). While in the European Union (EU) the decoupling between greenhouse gas emissions and chemical production has been significant in the past decades (EC, 2023), innovation is still crucial to continue decoupling the chemical demand trend from impacts on human health and the environment.

In the context described, the European Commission pursues the transition of the European chemical industry toward the production and use of safe and sustainable chemicals through the European Chemicals Strategy for Sustainability (CSS; EC, 2021b). Among the CSS planned actions, there is the development of criteria for Safe and Sustainable by Design (SSbD) chemicals, which aims to push for innovation in chemical sector—in particular, toward designing new chemicals and materials that are safe and sustainable, while improving the

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existing ones with the integration of a life cycle perspective. Several frameworks have been proposed in scientific and gray literature, as extensively reviewed and shown in Caldeira et al. (2022a). The review examined a total of 119 frameworks from different sources, including industry, academia, and governments. They were reviewed and mapped by type of product assessed (chemicals, material, service, etc.), the sustainability dimensions included (safety, environmental, social, and economic). This review contributed to the knowledge base needed for the subsequent work.

To support the development of the criteria for SSbD, the European Commission tasked its scientific support branch, the Joint Research Centre (EC-JRC), to create a framework that integrates four sustainability dimensions: safety, environmental, social, and economic (Caldeira et al., 2022b). As a result of this effort, the Commission adopted the JRC framework as a Commission Recommendation (EC, 2022).

The broad definition of environmental sustainability is responsible interaction with the environment to meet present human needs, avoiding depletion or degradation of natural resources for future generations, as described in the Brundtland Report (WCED, 1987). Since the Chemical Strategy for Sustainability calls for minimization of environmental footprint, climate change, pollution, and resource use from a life cycle perspective, Life Cycle Assessment (LCA) was chosen by the JRC as the methodology to support these objectives.

Life Cycle Assessment is a comprehensive method that accounts for all the stages of the chemical and material's life cycle and multiple environmental impacts, which allows for measuring impacts related to the four above-mentioned targets of the CSS. It also allows for the identification of tradeoffs between different stages of a product's life and various environmental impacts.

Life Cycle Assessment is used to support decision making in different cases. For the SSbD context, there are mainly two use cases of interest:

1) Evaluating the environmental performance of existing products to identify hotspot improvement or to compare alternative products. This case is related to the evaluation of potential substitution of an existing chemical or material with another existing one. Its relevance lies in the need to evaluate (ex post) current products.
2) A second use is the anticipatory assessment of potential impacts of emerging technologies (ex ante LCA) or to project current and incoming technologies onto future scenarios (prospective LCA). This case is highly relevant to SSbD due to its expected adoption "in research and innovation activities related to chemicals and materials" (EC, 2022).

Regarding the first case, LCA has been extensively used in the past to evaluate the environmental performance of chemicals. Burgess and Brennan (2001) reviewed the application of LCA to chemical processes rather than products, asserting its relevance for process design and optimization in order to recognize environmental hotspots and potential improvements. Jiménez-González and Overcash (2014) focused on the pharmaceutical sector; they provide practical suggestions for LCA practitioners and also call for more transparency on the LCA underlying assumptions and sharing of data in the sector to increase the availability of secondary data for other practitioners. An extensive review on the use of LCA for chemicals in scientific literature has been performed by Santos et al. (2019) screening the studies by different criteria, such as the database and software used, impact categories assessed, and system boundaries definition. The authors observed a focus on climate change, while other impact categories received less attention in the reviewed literature. For example, for human toxicity, the most used health-related impact category, only 37% of the studies were using it against the 93% of them for climate change, with 20% of the reviewed considering only this impact category. This bias toward climate change undermines a fundamental strength of LCA: Its capacity to prevent burden shifting—the phenomenon where improvements in one impact category lead to worsening impacts in others. Moreover, a severe lack of uncertainty analysis is reported (only six studies out of 46 had an uncertainty analysis). Kleinekorte et al. (2020) reviewed the use of LCA in process design, showing that two decades after Burgess and Brennan (2001), LCA is an established methodology applied to chemical processes and supply chains; however, they also highlight the need for better commercially available LCA data and the need to quantify the uncertainty of data gap filling methodologies.

In the anticipatory assessment, major challenges in LCA application are the difficulties related to availability and scaling up of primary data—that is, data collected directly from the specific process or technology under assessment—from pilot scale to industrial production volumes, or the uncertainty introduced by the technological evolution (e.g., new energy generation technologies), which affects the modeling of background systems (i.e., the part of the life cycle that is not under the control of the LCA practitioner, such as electricity generation, and therefore modeled using secondary data). Data scarcity and uncertainty may affect the reliability of assessment results.

Cucurachi et al. (2018) reflected on the importance of LCA application to emergent technologies, and its peculiarities compared to the LCA application to incumbent products and technologies, such as the need to define the function of an emerging technology, and adapt the comparison with an incumbent technology every time the innovation cycle leads to a change in functionality of the new one. While they discussed and acknowledged the issues of data availability and their uncertainty for ex ante LCA, they are also convinced that a transparent communication of assumptions and uncertainties can in any case direct the development of new technologies. Hetherington et al. (2014) analyzed three case studies of emergent technologies, including one on carbon nanotubes and one on fuels from lignocellulosic biomass, to outline challenges related to the use of LCA in early-stage research, listing scaling issues and data availability among the main ones. To address the challenge of modeling future technological scenarios, Sacchi et al. (2022) developed a method and a tool (Premise). It adapts existing LCA databases for use in prospective LCA studies changing the modeling of energy-intensive industrial processes according to projected scenarios for global energy systems. Thonemann et al. (2020) reviewed the applications of prospective LCA to technologies or systems of technologies in scientific literature to highlight challenges and proposed a general framework for conducting prospective LCA. Specific provisions for prospective and ex ante LCA in

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biotechnology processes are described in Wowra et al. (2023), stressing the importance of using LCA as a comprehensive methodology rather than simpler but incomplete metrics.

Overall, the mentioned studies show the wide use of LCA for environmental assessment of existing and emerging chemicals and materials and agree on the importance of data quality and availability for the application of LCA to the chemical sector.

The present study analyzes the first application of the Joint Research Centre (EC-JRC) framework. The selected case study considers a set of plasticizers for plastic materials used in a food contact application. Plasticizers are substances used to increase the flexibility and workability of polymers, and they are especially combined with polyvinyl chloride (PVC) to manufacture soft PVC products. A group of plasticizers called phthalates have been scrutinized in the past for safety concerns due to their migration from plastic materials in which they are used, leading to potential health risk. However, when looking for safer alternatives, the environmental aspects related to the life cycle impacts received significantly less attention, showing the need for an approach that integrates safety and environmental sustainability. For this reason, this class of chemicals has been selected for the case study.

The objective of the paper are (1) to present the results of the case study on plasticizers; (2) to state and discuss the challenges in the use of LCA that emerged during the case study, and that are applicable to the broad scope of the SSbD framework, to support it; and (3) to discuss possible ways to address them and highlight future topics for the scientific community to contribute to. The study builds on the case study presented in Caldeira et al. (2023), delving into methodological issues related to the LCA applications. Specifically, the case study identifies the challenges of LCA that arise in the use of the SSbD framework. While some of the challenges are already discussed in LCA scientific literature, as presented in the *Introduction*, in the present study they are analyzed also under the SSbD angle. The SSbD is tested evaluating the applicability of the framework to plasticizers used for food contact applications.

Methods

To facilitate the identification of challenges for the implementation of the LCA in the SSbD, methods are presented in two sections: an overview of the SSbD framework with a focus on the use of LCA for the assessment of environmental sustainability, and the description of the approach adopted to develop the case study following the structure of LCA phases.

Safe and Sustainable by Design (SSbD) framework

The framework developed by the JRC has the goal to support and operationalize the SSbD approach by setting a methodology for the assessment of safety and sustainability aspects of chemicals, providing guidance on criteria for the definition of SSbD chemicals and hence enabling their performance-based comparative assessments. The original framework (Caldeira et al., 2023) has been recently updated and published (Garmendia Aguirre et al., 2025). However, the environmental sustainability part is relying always on LCA.

The framework is articulated in different phases: the safety part, which addresses hazard assessment of the chemical based on its intrinsic properties, exposure to the chemicals, and the sustainability part, the focus of this study, addressing environmental sustainability and the potential environmental impacts of the chemical along its life cycle using the LCA. The LCA part considers 16 impact categories. The overall ambition of the framework is also to aggregate these different aspects in a scoring system that allows the comparison of different chemicals (or different production processes for the same chemical) and to set criteria to define if they are safe and sustainable. The former implies the definition of reference values for each aspect to compare the assessed chemicals. The reference is then used to derive a score for each environmental sustainability aspect of the framework.

The calculation of the SSbD score is envisioned in the framework for the environmental sustainability assessment and tested in the present case study. It is derived from the results of the LCA and reflects the degree of improvement (i.e., reduction of impacts) of a product's environmental sustainability performance relative to a reference value. In the present case study, the environmental performance of one of the plasticizers was used as a reference.

The proposed scoring system for the sustainability assessment uses a scale from 0 to 3, as presented in Table 1. A score of 3 is given when the alternative product presents significantly lower impacts (>20% improvement) than the reference product, 2 for reduction in impact between 5% and 20%, and 1 when the chemical presents impacts similar to the reference. Finally, a score of 0 is given when the chemical is significantly worse than the reference. Then, the 16 impact categories were grouped into the above-mentioned four groups (toxicity, climate change, pollution, and resource use), and the scores were averaged into a final environmental sustainability score. Then, these scores were used for the aggregation with safety scores coming from the other steps of the assessment. Since this part of the framework is out of the scope of the present article, it will not be discussed here. The proposed scoring and aggregation system shown in Table 1 is not part of the existing framework, since it was defined specifically for the case study. Hence, the final choice on the scoring and aggregation method is left open.

Case study description

Goal and scope of the LCA

The case study refers to the application of the LCA part of the SSbD framework to a set of six plasticizers used in food contact material in Europe, namely:

- Di(2-ethyl hexyl) phthalate (DEHP)

Table 1. Scoring system tested for the sustainability assessment of an alternative plasticizer versus the di(2-ethyl hexyl) phthalate reference.

Percentage change of improvement in impacts of the alternative (%)	Score for impact categories
≤ −10%	0
−10% – +5%	1
+5% – +20%	2
>20%	3

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- Di(2-ethyl hexyl) terephthalate (DEHT)
- Di(2-ethyl hexyl) adipate (DEHA)
- Di(isononyl) cyclohexanoate (DINCH)
- Acetiltributylcitrate (ATBC)
- Epoxidized soybean oil (ESBO)

A phthalate plasticizer, DEHP, is included to be used as a reference material, considering its widespread use in the past in PVC for several applications, from flooring tiles to food packaging. The other five plasticizers, here considered as potential substitutes for DEHP, are selected considering the most common nonphthalate plasticizers from different chemical feedstock to test different supply chains, among the ones allowed for food contact according to European regulation (EC, 2011). To set a complete cradle-to-grave LCA, the plasticizers must be evaluated for their application in a product. Hence, they are considered for their use in a specific packaging application: the manufacturing of PVC-based gaskets for metal lids. This choice allows us to define a use phase and an appropriate end-of-life scenario, completing the life cycle. The entire life cycle of the product is considered to happen in Europe.

The Product Environmental Footprint (PEF) method (EC, 2021a) is used as a methodological reference. The PEF method prescribes the use of specific rules for different products defined by documents called Product Environmental Footprint Category Rules (PEFCR). Since no PEFCR exists for chemicals or plasticizers, the default methodological provision of a PEF study is applied.

The functional unit of this study is 1 kg gasket, able to act as an airtight seal between the glass jar and its metal cap, and to guarantee the whole shelf-life of the food contents of the jar, which is suitable for contact with oily food. Then for each gasket a specific formulation is set with different shares of PVC, plasticizer, and other additives (e.g., stabilizers, pigments). The original formulation, based on DEHP, has been adapted to the other plasticizers using a substitution factor based on the ability of each plasticizer to give the compounded PVC a defined level of hardness (Godwin & Krauskopf, 2008). For example, for ATBC, the substitution factor of 1.06 means that the amount of ATBC will be 1.06 times the DEHP. Substitution factors and composition are reported in Table 2.

Life Cycle Inventory (LCI)

The modeling of the life cycle is performed using different sources of data: academic literature from the industrial chemistry and polymer manufacturing field, computer-aided process simulation, existing LCA models, and national statistics.

Table 2. Substitution factor used to calculate the amount of plasticizer compared to the DEHP (reference) and mass-based compositions of each gasket calculated using the different plasticizer used and substitution factors used to derive them.

Composition	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Substitution factor	1	1.06	0.93	1.03	1.09	1.1
Plasticizer (%)	35.8	37.2	34.2	36.5	37.8	38.0
PVC (%)	47.8	46.8	49.0	47.2	46.3	46.1
Other additives (%)	16.4	16.0	16.8	16.2	15.9	15.9

Note. DEHP = di(2-ethyl hexyl) phthalate; ATBC = acetyltributylcitrate; DEHA = di(2-ethyl hexyl) adipate; DEHT = di(2-ethyl hexyl) terephthalate; DINCH = di(isononyl) cyclohexanoate; ESBO = epoxydized soybean oil; PVC = polyvinyl chloride.

For the modeling of raw material production, literature data on the synthesis of the chemical precursors of the plasticizers were used to model the related foreground processes and link them with the LCA datasets chosen from the background databases (Ecoinvent 3.6), using the software Simapro. Information on the synthesis of the plasticizers and their precursors come from *Ullmann's Encyclopedia of Industrial Chemistry* (Wiley, 2003).

Plasticized PVC is manufactured creating a solid suspension of PVC in liquid plasticizer, called plastisol. Data on the manufacturing technology of plastisol and the manufacturing of the gasket are retrieved from Bayer et al. (1988) and Giessler and Ratliff (1968), additionally confirmed by industrial stakeholders.

After collecting information on the industrial processes from the literature, some data gaps are filled using process design software—in particular, to estimate the energy input in the synthesis of ATBC—while in the case of ESBO, the literature is complemented by the information retrieved from an ESBO manufacturer (Hairma (Nantong) Technology, 2022). Details on the modeling and complete life cycle inventories are presented in the Annex 7 of Caldeira et al. (2023). For one, DINCH, an LCI of its precursor (di-isononyl phthalate, or DINP) is available (ECPI, 2015), and it is manually mapped from the ILCD (International Reference Life Cycle Data System) nomenclature of elementary flows to the one used in the LCA database Ecoinvent.

The end-of-life of the plasticizer is built considering the disposal scenario of the cap, since the gasket is not separated and the plasticizer is mixed with the PVC. Lacking specific information on this waste fraction, the end-of-life scenario is modeled considering the average European share of landfill and incineration for municipal solid waste (Eurostat, 2022). Specific disposal datasets for each plasticizer and the PVC additives have been developed for all the plasticizers, using the indication and tool provided in Doka (2020).

Life Cycle Impact Assessment (LCIA)

Life Cycle Assessment impacts are calculated using the Environmental Footprint impact assessment method (version 3.1). This method was selected due to its comprehensive coverage of 16 impact categories at midpoint level (i.e., quantifying the impacts at the level of cause–effect chain of the impact, before the final effects on humans or the environment), encompassing all the relevant aspects of the framework, and is the method recommended by the European Commission in the application of LCA. The impact assessment method also includes toxicity-related impact categories, namely freshwater ecotoxicity and human toxicity (cancer and noncancer). These categories address potential safety-related concerns arising from the indirect exposure to all the chemicals along the life cycle and could affect humans and the environment through their diffusion in different environmental compartments (air, water, and soil).

Results and discussion

The results of the case study are presented in two subsections. The first presents the results of the LCA of the six plasticizers, and the second discusses the challenges identified during the development of the case study, considering their potential implications for LCA in the SSbD context. Starting from the case study, some of the challenges identified go beyond the specific case analyzed and can be generalized for the application of SSbD to the whole chemical industry.

Case study results

The impact assessment results of the six plasticizers for the 16 impact categories, calculated through the Environmental Footprint impact assessment method, are presented in Table 3. The impacts for the 16 impact categories are presented as percentage change between each gasket and the reference DEHP gasket. Hence, positive numbers represent a higher impact compared to the reference for that impact category. Results show that the impact of the different gaskets is close for several impact categories, mainly due to the commonalities in their life cycles, such as the plasticizers' precursors (e.g., ethyl hexanol for DEHP, DEHT, and DEHA) and the gasket manufacturing stage. However, for some impact categories, such as land use and marine eutrophication, there is a sharp difference between ATBC and ESBO and the rest of the plasticizers. These differences come from the use of biomass in the supply chain of their precursors (citric acid and soy oil), which cause higher impacts on these impact categories compared to the fossil-based plasticizers, including the reference. For the same reason, the use of a bio-based feedstock in ESBO shows a significant reduction in the fossil resource use (−31%). As described in the LCIA section and in Table 1, these results were used to calculate the SSbD score for environmental sustainability. The score for each of the four groups and the final aggregation can be seen in Figure 1 for all the plasticizers.

The results highlight the need for a decision-making methodology that allows for solving tradeoffs. While in the present case LCA results may be too similar in most instances to establish which alternative plasticizer is better, this is due to the use of literature rather than relying on actual data. Moreover, since the aim of the framework is to join safety and environmental issues, the final decision will be made considering also the outcomes of the other parts of the framework.

Challenges

In this section, the challenges encountered in the application of LCA in the SSbD context are discussed in relation to the case study, considering the goals of the CSS. Challenges are presented in the next subsections following the phase of the life cycle assessment to which they are related.

Goal and scope definition

Challenge 1: Benchmark selection

One of the requirements of the SSbD framework is to set criteria for the sustainability of chemicals; therefore, a benchmark is needed for each impact category. The most common way to address this aspect of LCA is to define the product as the basis for comparison for those with the same function. The chosen benchmark can represent the average performance of the group of products or the best in class. Many ways of defining a benchmark can be used, depending on the goal of the comparison, but they are all underpinned by the assumption that these products have a similar function for the end user. The similarity implies that products are mutually substitutable and thus comparable. This is explicitly required by both the ISO 14040 and 14044 standards and by the Product Environmental Footprint (PEF) methodology. The PEF, in addition, defines benchmarks

Table 3. Percentage improvement of the impacts for each plasticizer compared to the reference DEHP gasket and derived score. Positive percentages indicate a higher impact than the reference, and negative ones indicate lower impacts.

	Percentage (%)						Score					
Impact category	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Human toxicity, cancer	–	−18	−67	1	14	−37	1	0	0	1	2	0
Human toxicity, noncancer	–	−31	−9	0	11	2	1	0	1	1	2	1
Ecotoxicity, freshwater	–	−22	−4	1	6	−6	1	0	1	1	2	1
Climate change	–	−8	−36	1	−4	−32	1	1	0	1	1	0
Ozone depletion	–	−7	−7	0	12	11	1	1	1	1	2	2
Particulate matter	–	−23	−21	10	14	10	1	0	0	2	2	2
Ionizing radiation	–	−9	−1	0	−6	11	1	1	1	1	1	2
Photochemical ozone formation	–	−14	−9	8	8	9	1	0	1	2	2	2
Acidification	–	−28	−14	4	7	10	1	0	0	1	2	2
Eutrophication, terrestrial	–	−40	−16	2	5	−3	1	0	0	1	1	1
Eutrophication, freshwater	–	−17	−7	1	11	−1	1	0	1	1	2	1
Eutrophication, marine	–	−41	−10	3	6	−146	1	0	0	1	2	0
Water use	–	−49	−2	1	−2	0	1	0	1	1	1	1
Land use	–	−665	−8	1	6	−327	1	0	1	1	2	1
Resource use, fossil	–	−2	−6	2	−2	31	1	1	1	1	1	3
Resource use, minerals and metals	–	−40	−11	−3	13	−12	1	0	0	1	2	0

Note. DEHP = di(2-ethyl hexyl) phthalate; ATBC = acetyltributylcitrate; DEHA = di(2-ethyl hexyl) adipate; DEHT = di(2-ethyl hexyl) terephthalate; DINCH = di(isononyl) cyclohexanoate; ESBO = epoxydized soybean oil.

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Toxicity	Level
DEHP	1.00
ATBC	0.00
DEHA	0.67
DEHT	1.00
DINCH	2.00
ESBO	0.67

Climate Change	Level
DEHP	1.00
ATBC	1.00
DEHA	0.00
DEHT	1.00
DINCH	1.00
ESBO	0.00

Resources	Level
DEHP	1.00
ATBC	0.25
DEHA	0.75
DEHT	1.00
DINCH	1.25
ESBO	1.00

Pollution	Level
DEHP	1.00
ATBC	0.25
DEHA	0.50
DEHT	1.25
DINCH	1.75
ESBO	1.50

Environmental Sustainability Score	Level
DEHP	1.00
ATBC	0.38
DEHA	0.48
DEHT	1.06
DINCH	1.50
ESBO	0.79

Figure 1. Scores obtained by each gasket in the four impact groups defined by the Safe and Sustainable by Design framework and their final aggregation in a single score. DEHP = di(2-ethyl hexyl) phthalate; ATBC = acetyl tributyl citrate; DEHA = di(2-ethyl hexyl) adipate; DEHT = di(2-ethyl hexyl) terephthalate; DINCH = di(isononyl) cyclohexanoate; ESBO = epoxydized soybean oil.

for product categories inside the so-called Product Environmental Footprint Category Rules (PEFCR), which are not available for all the existing products and may not have the desired granularity.

When the goal of the innovation is to develop a brand-new chemical or a material with a defined function and a known market, without targeting the substitution of a specific chemical or material, it may be suitable to define a reference that represents the specific market segment. This approach follows the logic of the market average benchmark, which is the principle used to define benchmarks in the PEF method.

In the case study, the environmental impact of each gasket is compared to the DEHP gasket, which has been chosen as a reference since it is a general-purpose plasticizer that has been used in many applications before being phased out due to safety concerns. In this case, the comparability among gaskets is ensured by the definition of the functional unit, which defines the quantitative basis for the comparison at the product level (for the case study defined in the *Methods* section) and the method used to calculate the composition of the different gaskets. The study simulates the case in which a company wants to find an alternative to an existing chemical.

In both cases, these approaches allow for measuring an improvement of environmental performances against an existing situation (i.e., the substituted chemical).

A different way to set a reference value in the SSbD context would be to link the environmental impacts with the Planetary Boundaries (PB) framework (Rockström et al., 2009). This would allow us to move the comparison from relative sustainability (Chemical A is more sustainable than B) to an Absolute Sustainability Assessment (Chemical A is sustainable) and state that a chemical in a specific application leads to environmental impacts that are within the limits that the Earth system can withstand. An effort in this direction was made in Sala et al. (2020), in which a link between the PBs and the Environmental Footprint impact assessment method has been established, allowing the comparison of LCA results with the PBs. However, while the allocation of the PBs to countries can be done by attributing a share of PB that is proportional to population, allocation to products and in particular to chemicals is more difficult. An attempt for chemical commodities has been done by Tulus et al. (2021) using economic criteria. However, this approach does not currently appear scalable at the level of fine chemicals and is not able to consider the impacts arising from the specific function of a chemical in its final use and therefore does not cover the entire life cycle of a chemical.

Thus it is important for the application of the SSbD framework that a benchmark that is consistent with the goal of the innovation process is used, while the scientific community can investigate how to define absolute sustainability criteria.

Challenge 2: Assessment of intermediate chemicals/materials

Life Cycle Assessment is a decision-making methodology that can be used to evaluate alternatives. The functional unit shall be defined to compare and select alternatives. This choice is made in the SSbD framework to ensure that the full life cycle is evaluated and to avoid burden-shifting between different parts of a product's life (e.g., lower impacts during manufacturing can be compensated for by higher impacts during final waste treatment).

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The goal of the SSbD framework includes the ability to compare alternative chemicals also at the intermediate level and the definition of a reference value (see Challenge 1) for the impacts to define whether or not a chemical is SSbD. Moreover, it can be applied by different organizations along the supply chain, and this requires communication among them (e.g., the SSbD assessment of an intermediate chemical is used as input for the assessment of a final product by another organization). Therefore, a consistent way to deal with them is necessary. In the current work, it was possible to identify the following cases:

1) **Different chemicals**: SSbD is applied to one or more chemicals that can be used in different commercial applications. In this case, since each application may require a different technical performance from the chemical, each of them will determine a different functional unit and the SSbD assessment will be chemical- and application-specific. This is the case of the plasticizers case study, for which many applications are possible, but the gasket manufacturing was defined as the specific one assessed.
2) **Same chemical with different production process**: If the comparison is made between the same chemical obtained from different processes (hence different supply chains), then it is theoretically possible to establish a comparison at the intermediate level as well. In this case, whatever the final application is, both the chemicals will be equally able to fulfill it. It is important to note differences in the production process, which may lead to differences in properties that affect its use for the final application (e.g., as concentration, impurities, or color). Therefore, the technical equivalence between the chemicals (i.e., they can be perfectly substituted in all final applications) should be verified. An example is the assessment of a plasticizer derived from two different feedstocks, such as the production of ATBC from fossil-based and bio-based butanol. In this case, the cradle-to-gate assessments of the two different supply chains are comparable, since the intermediate product is the same and they can fulfill the same functional unit. Yet, they cannot be defined as safe and sustainable without a defined application that allows the assessor to consider the whole life cycle.
3) **Chemical as a precursor**: When a chemical is used as reagents for another reaction. In this case, the functionality provided is the ability to produce the desired final chemical and the life cycle ends with the use of the chemical as a reagent. Therefore, it can be considered a complete LCA instead of a cradle-to-gate assessment of an intermediate. For example, acetic acid and acetic anhydride can be assessed and compared in their use as acetylation of tributyl citrate.

For cases 2 and 3, it is important to highlight that there might be information in the chemical's cradle-to-gate inventory that is relevant for the next life cycle stages in a cradle-to-grave LCA—for example, the biogenic carbon content (since it affects the modeling of the end-of-life of the chemical in a product) or the content of substances that can be released during the use or the end-of-life of the product (see Challenge 5 and 7) and lead to environmental impacts. This information shall be documented clearly to allow the correct use of the LCA model of the intermediate chemical in other LCA. Therefore, even if from the LCA point of view it may be possible to establish meaningful comparison at an intermediate level, this is not sufficient from an SSbD perspective. However, the information on the assessment at the intermediate level is crucial for the modeling of other chemicals or materials downstream of the analyzed one, so it is important that cradle-to-gate assessments are used and passed along the supply chain up to the point where a final application, and hence a functional unit, can be defined.

Life Cycle Inventory

Challenge 3: Data availability in the chemical supply chains

The case study highlighted a long-standing problem with LCA: the availability of primary data across the chemical manufacturing value chain, which is hindered by its fragmentation and complexity and by data confidentiality concerns. In this case, a complex landscape of companies exists, ranging from the big petrochemical companies producing the commodity chemicals, to fine-chemicals companies, to formulators that mix different chemicals to create the final product. In 2024, according to ECHA, more than 22,000 substances are registered in Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) (ECHA, 2024).

Having an updated and technologically representative modeling of the chemical supply chain is crucial at this moment since many new technologies are entering the market to improve the environmental performance of the chemical industry (IEA, 2024). Moreover, since the goal of steering the sector is stated both by policymakers and industry (CEFIC, 2024; EC, 2023), developing updated LCA of chemicals is an effective way to track the improvement of the sector and to exchange data among companies, easing the task of performing LCA of their portfolios.

To address this challenge, data gap estimation procedures have been proposed in the literature. Parvatker and Eckelman (2019) and Wernet et al. (2012) proposed a ranking of data-gap filling methods, starting from the lowest accuracy (estimates based on molecular structures) to the best case in which primary data from a production plant are available.

However, some of these procedures, such as the use of proxy datasets (i.e., datasets of chemicals that are assumed to be similar to the targe ones) and the molecular structure-based models (SMS) may be considered as viable options only for the modeling of auxiliary chemicals in the life cycle, since they can be too inaccurate to represent the chemical under assessment.

For example, the use of proxy datasets is based on the assumption that two chemicals have strong similarities in their life cycle (Method 6 in the Parvatker and Eckelman, 2019 hierarchy). If this assumption is verifiable, and thus there is enough information on the chemical under assessment to conclude that it is similar to the proxy chemical, then it is likely that the known information can be used to build a basic model of the chemical in scope (Method 4 in Parvatker and Eckelman, 2019). On the other side, if the assumption cannot be verified, then it may introduce strong biases in the model.

Regarding SMS, they should be used with caution since they are based on the debatable assumption that the life cycle of a chemical can be inferred by its structure, while different chemical pathways or feedstocks can be used to achieve the same chemical structure. The missing causal relation in SMS is also pointed out by Langhorst et al. (2023). In contrast, they

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quantitatively compared a set of estimation models based on stoichiometry. However, the approach used by Wernet et al. (2012) to rapidly screen a set of chemicals in a complex mixture is a good example of how to deal with the tradeoff between accuracy and time resources used in modeling.

While these are currently valuable procedures to fill the gaps and highlight priorities in data collection, they will become increasingly far from reality in the upcoming years, when new emerging technologies will be implemented (e.g., electrification, use of alternative feedstock) or when the market condition changes in the oil market. For example, the development of shale gas fields in the United States led to a significant increase in the ethane cracking capacity (to produce ethylene) in the period 2014–2017, and to additional export of this feedstock to Europe and India (IEA, 2019). This kind of technological change can lead to meaningless LCI in the following years or to poor applicability of data gap-filling techniques, especially when the technological change affects the production of chemical commodities such as ethylene (IEA, 2018, 2023).

A key role in fixing this challenge can be played by industries and sectorial associations. Associations can gather the efforts from their members and become promoters of the development of specific product category rules, currently missing for many chemical groups. Chemical companies, particularly the ones producing commodity chemicals, can develop and share LCA profiles for their product. In this way, they will significantly improve the quality of secondary data available to researchers and downstream companies, also reducing the effort required by the sector to apply the SSbD framework. In addition, the publication of base chemicals LCA will reduce the cost of developing new LCA profiles for fine chemicals. The increase in the number of public LCA profiles for chemicals will also be beneficial to build extensive databases to train machine learning algorithms.

Challenge 4: End-of-life scenarios

Following the issue of data availability in the chemical supply chains, a similar lack of data exists for the downstream stages of a chemical or material, end-of-life in particular. For example, in the case study, the emissions due to the incineration of the plasticizers, the PVC, and the additives were modeled under the assumption of average waste treatment. No specific information was available on the disposal of the waste fraction of metal caps, or a similar one. However, modeling the emissions of the plasticizers themselves into the environment would require several assumptions on the migration dynamic of the plasticizers from the PVC matrix and to air or water. In the SSbD context, this modelization can be done following the assessment of consumers' and workers' exposure, which is part of the safety assessment and modeling of the framework.

However, also to do so, the emitted chemical shall exist in the list of available elementary flows and have a characterization factor in the LCIA method. Otherwise, the inclusion of this emission in the LCI does not affect the final results (see Challenge 7). For the described reasons, in the SSbD application, the fate of the chemical or material in the specific application considered can be hard to track, for the following reasons:

1) The company manufacturing the chemical or the material does not have specific information on the fate of its product after its use by the consumer.
2) The granularity of statistics on waste may be insufficient to model an appropriate end-of-life scenario. Additionally, waste treatment differs substantially in different countries, both in shares of disposal and recovery and in technology used; thus regional considerations might be needed for a realistic representation of the waste management and treatment. An interesting approach that can be used to model specific scenarios is to use material flow analysis at the country/regional level to derive information for LCA modeling. Since this type of analysis usually joins statistics and data from different sources, together with specific knowledge on the collection and treatment of waste, it derives a more detailed model of the mass flows of waste in a sector (Amadei et al., 2023).
3) Then, each chemical may lead to different emissions into nature due to its migration or due to chemical reactions occurring, such as the combustion of the chemical in a waste treatment plant. While emissions due to the incineration process can be often modeled assuming complete combustion and stoichiometry (Doka, 2020), it is more difficult to model the release of the chemical into air, water, or, soil in other waste disposal treatments.

Challenge 5: Additional information on material and elementary composition in LCI

The mathematical structure of LCA is based on unit processes that are built as a list of input and output needed to produce one unit of a product; therefore, the unit processes can be represented as vectors of numbers expressing the amount of each input/output required. Those inputs/outputs can be either the product of other unit processes (technical flows), a natural resource extracted from, or a substance emitted to, the environment (elementary flow). This type of data structure is convenient for the calculation of environmental impacts that are reduced to the operation of solving a linear system (Heijungs & Suh, 2002). However, this data structure loses other information about the unit process, which can be relevant in other parts of the life cycle.

For example, in the plasticizer case study, two plasticizers have a biogenic carbon content due to their precursors, namely the ESBO obtained from the soy oil and the ATBC from the citric acid, which is currently produced with a fermentation process of biomasses. The information on the carbon content was then used to model the emissions in the incineration process accordingly. However, the detailed modeling of carbon input to the incineration process, further converted to energy and emissions, was possible because of the relatively short supply-chain and the documentation available for the secondary datasets and since the entire cradle-to-grave assessment was performed by the same practitioner. In the case of more complex supply chains, this information may be lost in the background model and therefore not accounted for properly at the end-of-life stage (see Challenges 4 and 7).

A more consistent way to address this issue would be to embed this information into the LCA data structure, as is done with uncertainty parameters or geographical location. A step in this

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direction is the development of a more complex data structure, namely an ontology for LCA data, which will define additional properties of a dataset that can be later used for automatic calculation (Ghose et al., 2022).

Challenge 6: Innovation prospective and ex ante LCA
The SSbD is a premarket approach able to drive sustainable innovation in the chemical industry (EC, 2021b). In particular, it is meant to be a framework to provide guidance during the development phase, to evaluate different environmental impacts, and to be incorporated in the usual research and development activities of companies. While LCA is an already established method among companies to evaluate existing processes and technologies, it is often used in academia to evaluate emerging technologies. When studying a new technology, one objective could be to estimate its environmental impacts when it matures, such as when it is commercialized and produced at an industrial scale. Another objective might be to assess the technology's potential impacts in the future, considering the evolving technological landscape. The first approach is often called ex ante LCA, while the second is named prospective (Arvidsson et al., 2024). Both these approaches are very relevant for the SSbD due to the before-mentioned goals. Since different applications often lead to very different scenarios and assumptions, it makes it more difficult to compare results and properly interpret them.

In particular, when performing a prospective or ex ante LCA, the practitioner has to face practical issues:

Definition of a goal and scope that is consistent among different applications:

1) Lack of data to compile an LCI that is representative of the process at industrial scale
2) Scenario definition for relevant technological changes in time
3) Consistency of the foreground scenario assumed with the background datasets available
4) Difficulties in modeling the whole life cycle at an early stage of development

Guidelines for consistent methodological choices are strongly needed to support the practitioners in dealing with these aspects. While an example has been developed addressing bio-based products (Cucurachi et al., 2022) guidance should be extended to the rest of the chemicals and materials to facilitate SSbD application. Other examples of application of the prospective LCA have been performed on specific chemicals such as aniline (Winter et al., 2021) or adipic acid (Aryapratama & Janssen, 2017), which show the differences in approach that can be used in the modeling. Sacchi et al. (2022) developed a methodology to adapt the existing LCA database to future scenarios. While this approach can be extremely useful, it currently requires of the practitioner additional programming skill, which hinders the usability, especially outside of academia.

Moreover, different types of innovation can take place in the chemical industry, and they need different approaches. While sometimes a brand-new chemical is designed having in mind its desired function (e.g., a pesticide), in other cases it may be necessary to find a suitable process to valorize a given feedstock, turning it into a more valuable chemical (e.g., valorization of a by-product).

Life Cycle Impact Assessment

Challenge 7: Impacts from substances of concern
One of the important goals of the SSbD is to reduce the use of substances of concern (SoC), not only considering them as a direct object of the assessment but also analyzing the substances involved in the life cycle of a chemical or material that does not possess the hazard properties itself. To implement this life cycle perspective, LCA has to face three challenges:

1) Characterization factors for SoCs must be developed and included, where missing, in the impact assessment models to take into account their potential environmental impacts.
2) Their presence in products or materials shall be included and reported clearly in background datasets, to allow proper modeling of the end-of-life from the practitioner side, when this information is not available. Indeed, if no information on the presence of a plasticizer is present in the background data, then it will not be possible to model its release in the environment while modeling the end of life of the building.
3) The manufacturing of substances of concern should be covered in LCI databases. While they may be minor constituents in final products, and hence tend to be overlooked or cut off in performing LCA of complex products, they may be relevant for toxicity impact categories. Moreover, since some of them, like plasticizers, are commonly used as additives in many different materials (e.g., plastics, paints), the lack of inclusion in background datasets may lead to an underestimation of impacts in many products that are downstream of the chemical sector domain (e.g., construction or automotive).

The relevance of this aspect relates to the communication of SSbD results (and hence LCA) along the supply chain. For example, considering the use of PVC gaskets in the food industry, if the manufacturer of plasticized PVC uses a small amount of a SoC in its formulation (as an additive or an impurity), then the information shall be available to the gasket manufacturer. This data exchange will help the manufacturer to include it in its LCA and SSbD assessment and properly account for impact arising from the possible migration of the SoC during the use or end-of-life of the final product.

Conclusions and outlook

In the European Union, the concept of safe and sustainable chemicals gained attention since the publication of the Chemical Strategy for Sustainability by the European Commission. Since then, the attempts to consider both safety and environmental sustainability in the chemical industry were mostly theoretical or application specific. The publication of the SSbD framework and related guidance provided a practical approach to facilitate the application of the concept.

The study has presented a comprehensive analysis of the challenges and opportunities associated with integrating LCA into the SSbD framework for chemicals and materials. The case study, focusing on plasticizers used in food contact applications, illustrates the methodological complexities and data limitations inherent in such assessments, which are articulated in seven identified challenges.

Three challenges (Challenge 1, 5, and 6) show that LCA methodology with specific advancements and standardization would be able to address the challenge of benchmark selection and the application of the framework to innovative technologies. Indeed, while existing rules allow for defining comparative benchmarks to measure if a chemical is better than another in the chosen application, it is still impossible to understand if the chemical itself can be defined as sustainable on an absolute scale. An advancement in the field of absolute sustainability would be needed to operationalize the application of the Planetary Boundaries framework to individual chemicals. Besides, improving the data structure of LCA would vastly increase the exchange of data between organization and the automation of LCA analysis.

Moreover, the application of SSbD to innovative technologies to produce chemicals requires consideration and tools different from the ones used in ex post LCA, which is the scope of the Product Environmental Footprint methodology and the most common application of LCA. However, the scientific community is particularly active in defining methodologies and developing tools for the application of LCA to emerging technologies. This effort can be leveraged to make the SSbD framework more actionable in early stages of innovation, as described in the revised recommendation.

The remaining challenges (2, 3, 4, and 7) are not related to a methodological lack in LCA; rather, they call for an improvement in the way LCA data are produced, organized, and shared. The more new datasets on chemical supply chains are made available, the easier it is to create new LCA datasets for other context/cases/stakeholders. A combined effort between industry and academia may be useful to address the lack of data on the end-of-life, for example by combining the information from the industry with more advanced approaches from academia, such as material flow analysis.

In conclusion, while the integration of SSbD and LCA presents significant challenges, it is a crucial step toward ensuring the safe and sustainable development and use of chemicals, since the LCA is the only methodology that can evaluate various impacts along the entire supply chain of a chemical (as requested by the Chemical Strategy for Sustainability).

Data availability

The data related to the life cycle inventories and life cycle impact assessment are publicly available in the JRC repository at: https://doi.org/10.2760/329423.

Author contributions

Davide Tosches (Conceptualization, Formal analysis, Methodology, Writing—original draft, Writing—review & editing), Carla Caldeira (Conceptualization, Methodology, Writing—review & editing), Francesca Demichelis (Conceptualization, Writing—review & editing), Debora Fino (Conceptualization, Supervision, Writing—review & editing), and Serenella Sala (Conceptualization, Methodology, Supervision, Writing—review & editing)

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Conflicts of interest

None declared.

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