Doctoral Dissertation
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Life Cycle Assessment as support to Safe and Sustainable by Design

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Summary

This doctoral thesis explores the integration of Life Cycle Assessment (LCA) methodologies into the Safe and Sustainable by Design (SSbD) framework, focusing on the chemical sector. As SSbD aims at guiding innovation in chemical industry, robust and adaptable sustainability assessment tools become essential. The thesis addresses methodological challenges through four core chapters, each contributing to the practical application and advancement of LCA in SSbD contexts.

Chapter 1 presents the application of the SSbD framework to a case study involving six Polyvinylchloride (PVC) plasticisers used in food contact materials. The author contributed to the environmental sustainability assessment using the Product Environmental Footprint (PEF) method within an LCA framework. The study highlights limitations in data availability and methodological challenges when applying LCA to the SSbD framework.

Chapter 2 investigates the topic of comparability of LCA results for chemical products. By analysing the role of chemical nomenclature, intermediate classification, and dataset structuring, the chapter identifies the need for harmonised descriptors and system boundaries to enable meaningful comparison across substances. These findings are crucial for supporting alternative assessment within the SSbD framework.

Chapter 3 introduces a methodology to construct proxy processes for chemicals lacking detailed life cycle inventory (LCI) data. The tool maps synthetic pathways based on mass balances, allowing practitioners to trace back a substance's supply chain and build representative proxies. This method facilitates

screening-level assessments for data-scarce or emerging substances, a frequent need in SSbD evaluations.

Chapter 4 applies an advanced LCA modelling approach to assess the environmental impact of European plastic consumption under different trade and energy mix scenarios. By incorporating import data and future-oriented energy transitions, the study adapts Ecoinvent datasets to reflect changes in electricity and heat generation both geographically and temporally. This work supports prospective assessments aligned with EU policy goals and sustainability transitions.

The thesis overall contributes to the enhancement of LCA as a flexible, forward-looking tool for SSbD. It addresses the limitations of existing datasets and methods, offering practical solutions through data adaptation, proxy creation, and scenario modelling. These contributions are directly applicable to policy development, sustainability screening, and innovation processes in the chemical and material sectors.

Acknowledgment

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Introduction

In 2019, the European Commission published the European Green Deal (EC, 2019). A vast piece of policy that aims at making Europe the first climate-neutral continent by 2050. It is a blueprint for transforming the EU's economy to achieve sustainability, focusing on reducing carbon emissions, promoting renewable energy, and fostering a circular economy also in agreement with the Sustainable Development Goals set by United Nations. Its goals extend beyond environmental protection to include economic and social sustainability, creating green jobs, and ensuring a just transition for all sectors of society. By combining climate action with economic growth, the Green Deal aims to reshape industries, improve public health, and ensure a cleaner, more resilient future for Europe.

Among these goals, the protection of public health and environment are included as a part of the sustainable development.

One of the objectives of the Green Deal is the Zero Pollution Ambition, which aim to reduce levels of pollution in the environment below harmful levels by 2050. To do so, the EC set up a Chemical Strategy for Sustainability (CSS), which aims at creating a toxic-free environment and ensuring that chemicals are produced and used in ways that are safe for both human health and the environment. The CSS seeks to address the risks posed by hazardous chemicals while fostering innovation for safer alternatives. Its main objectives include reducing the presence of harmful substances, enhancing the control of chemicals, promoting the use of safe chemicals in everyday products, and supporting the transition toward green and sustainable chemistry.

In particular, by implementing the concept of developing a framework for the definition of Safe and Sustainable by Design criteria for chemicals and materials.

The Joint Research Centre (JRC) was tasked by the European Commission to develop this framework. As part of this effort, the JRC, in collaboration with Politecnico di Torino through the Collaborative Doctoral Programme, initiated a PhD project, which led to the work presented in this thesis.

The focus of this research was to apply Life Cycle Assessment (LCA) to develop and test the environmental sustainability assessment within the SSbD framework and provide support with upcoming implementation challenges. Over the course of the PhD, the framework was developed to provide a comprehensive assessment of environmental sustainability and safety. This process involved engaging with a wide range of stakeholders from both academia and industry to incorporate their feedback.

During the course of the PhD, the framework was created with the attempt of being comprehensive in the evaluation of Environmental Sustainability and Safety assessment. The development was a joint effort between two teams of researchers

with expertise in both domains and included listening to the suggestions and concerns of many stakeholders, both from academia and from industry.

Among the stakeholders' engagement activities two workshops were organised with my involvement and a 2-day workshop. After the framework was published in 2022, it was started to test it on a group of chemicals, with the goal of understanding the applicability of the framework, possible improvements and to provide support to external stakeholders willing to apply it.

From this test, a set of challenge were identified regarding the use of LCA and discussed in Chapter 1.

Chapter 2 to 4 presents discussions and exercises to answer some of the challenges presented in the first chapter.

Chapter 1

1 Role of LCA in the Safe and Sustainable by Design: lessons learnt from a case study

Food contact materials (FCM) are material meant to be in close contact with food such as those used in food packaging. They are essential along the food industry due to their ability in preserving food from deterioration due to physical, chemical and microbiological hazards. Several materials including plastics, rubbers, paper and metal, as well as their additives, such as plasticisers can be found in the food packaging materials. These materials are subject to several studies and investigation since they may migrate to or release other hazardous substances into food, posing health concerns to the consumers.

Plasticisers are among the most common additives for polymers, as they can make rigid plastics flexible or ease the shaping of a wide variety of polymers, such as polyvinyl chloride (PVC) or polyethylene terephthalate (PET). They are used in percentage ranging from 10% up to 60% by weight, according to the desired final properties of the polymeric compound.

For these reasons, the first application of the SSbD framework developed is the assessment of plasticisers in FCMs, in particular in the sealing gaskets of glass jar lids.

Plasticisers are extensively used to increase the flexibility of polyvinyl chloride (PVC). Soft PVC is widely used in such gaskets. The present case study examines the potential substitution of di(2-ethyl hexyl) phthalate (DEHP), currently labelled as a substance of very high concern (SVHC) due to its toxicity and endocrine-disrupting properties.

Among the potential alternatives, this study evaluates non-phthalate plasticisers. Namely, acetyl tributyl citrate (ATBC), di(2-ethyl hexyl) adipate (DEHA), di(2-ethyl hexyl) terephthalate (DEHT), di-isononyl cyclohexanoate (DINCH), and epoxidised soybean oil (ESBO). The goal is to apply the Safe and

Sustainable by Design (SSbD) framework to a realistic case study to test the feasibility of the assessment of safety, health, and environmental impacts of these alternatives compared to DEHP.

This chapter in particular is focused on the so-called Step 4, which assess the environmental sustainability of the gaskets.

1.1 Goal and Scope

The scope of the LCA is to compare different gaskets in a selected application (gasket for metal lids in food packaging), manufactured using different plasticisers, and to investigate which data are required and their influence on the application of LCA in the SSbD context.

The functional unit defines the quantitative and qualitative aspects that a product under assessment should provide. According to the PEF method (EC, 2021a), the functional unit shall be described considering the following aspects:

- The function(s)/service(s) provided: "**what**";
- The extent of the function or service: "**how much**";
- The expected level of quality: "**how well**";
- The duration/lifetime of the product: "**how long**";

The functional unit in this study is defined by the role of the product in which the plasticiser is applied. This approach enables a cradle-to-grave LCA, allowing for a fair comparison between alternatives. The selected product is a gasket for metal caps, and the functional unit is its ability to form an airtight seal (what), between a glass jar and its cap (how much), maintaining this seal throughout the shelf-life of the food contained the jar (how long), and being suitable for contact with oily food and allowed in FCM regulations (how well) (EC, 2011). A schematic depiction of the object is shown in Figure 1.

The reference flow is defined as the quantity of product necessary to fulfil the functional unit, which, in this case, is one gasket. However, since the choice of plasticiser does not affect the size or weight of the gasket, the reference flow can be expressed as a mass of gaskets, such as 1 kg, corresponding to a certain number of identical gaskets.

On another end, the plasticiser selection affects the composition of the gasket, with each plasticiser present in varying concentrations due to differences in their plasticising properties. It is important to note that the gasket's function is tightly connected to the function of the plasticiser, as the primary role of the plasticiser is to modify the properties of the PVC to meet the technical requirements for the gasket.

When combined with PVC, plasticisers convert the rigid resins into a softer compound which can exhibit a wide range of properties depending on the type and concentration of plasticisers used (Arkema, 2013).

The selection of a plasticiser for the formulation of the plastisol, a suspension of PVC particles and plasticiser, requires the balancing of different technical properties and parameters of the final compounded PVC.

For the application, among all the properties, the key technical property is the plasticiser efficiency in softening the PVC for the gasket application. This efficiency can be measured through the hardness of the final compounded PVC.

In particular, Shore A scale is used to measure the hardness of this type of materials (ASTM, 2021). The Shore A hardness identified for this application ranges between 60 and 80; the average value of 70 was chosen as the reference. Then, for each plasticiser a substitution factor was retrieved from literature, allowing the compounding recipe to be adapted from one plasticiser to another (Grossman, 2008).

Based on this measure, the substitution factor shown in Table 1 represents the quantity of a plasticiser needed to soften the PVC at the same hardness, compared to the quantity of a reference plasticiser (DEHP). For example, given the original formulation based on DEHP, a substitution factor of 1.06 for ATBC means that it is required to add 6% more it compared to DEHP, leaving all the other components (PVC and additives) unchanged. The composition reported in Table 1 are calculated based on the original formulation retrieved from Bayer et al., (1988); Giessler & Ratliff, (1968).

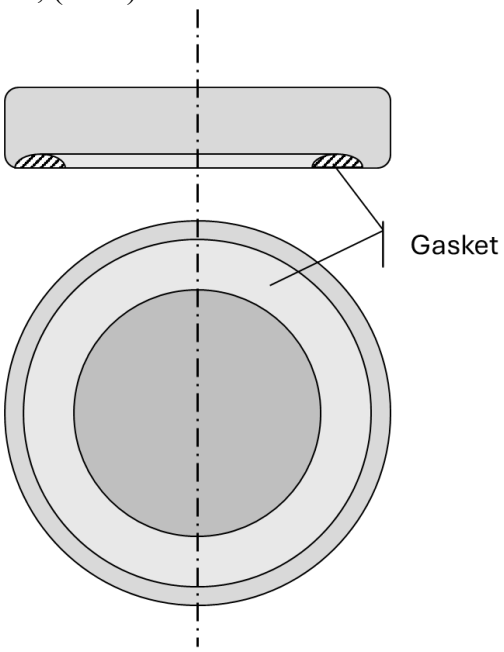

Figure 1. Schematic depiction of a metal lid (dark grey) with the plasticised polyvinylchloride gasket (light grey)

Table 1. Composition of the gasket with each plasticiser, with substitution factor used to calculate the different compositions

Component	**Di-(2-ethyl hexyl) Phthalate**	**Acetyl tributyl citrate**	**Di(2-ethyl hexyl) Adipate**	**Di(2-ethyl hexyl) Terephthalate**	**Di-isononyl cyclo-hexanoate**	**Epoxydised soy bean oil**
Substitution factor	1	1.06	0.93	1.03	1.09	1.1
Plasticiser	35.8%	37.1%	34%	36.5%	37.8%	38.0%
PVC	47.7%	46.7%	49%	47.2%	46.2%	46.0%
Blowing Agent (Na_2CO_3)	0.6%	0.6%	1%	0.6%	0.6%	0.6%
Stabiliser	1.2%	1.2%	1%	1.2%	1.2%	1.2%
Lubricant (stearic acid)	4.1%	4.0%	4%	4.0%	3.9%	3.9%
Pigment (TiO_2)	0.6%	0.6%	1%	0.6%	0.6%	0.6%
Filler (calcium carbonate)	10.0%	9.8%	10%	9.9%	9.7%	9.7%

1.2 Life cycle inventory

In this section is described how is modelled the Life Cycle of each of the six gaskets. The structure of the section follows the structure of the life cycle stages used in the PEF. The system boundaries considered are shown inFigure 2. The software used for the LCA modelling is Simapro. For secondary dataset, the Ecoinvent version 3.6 was used (Wernet et al., 2016)

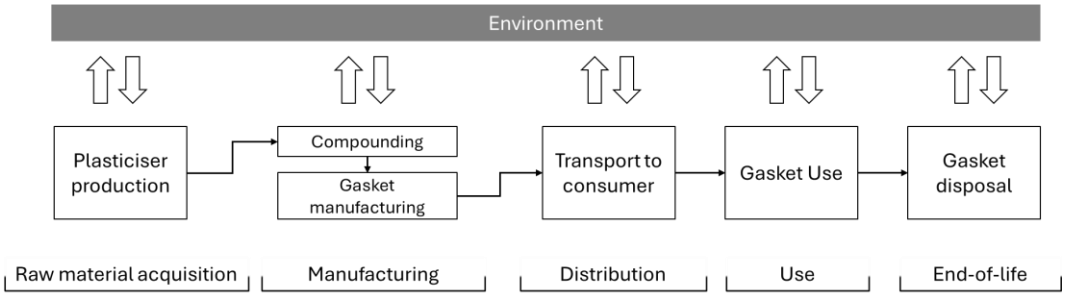

Figure 2. System boundaries of the Life Cycle Assessment with life cycle stages according to PEF method

1.2.1 Raw Material Acquisition and pre-processing

This life cycle stage includes all processes related to the production of raw materials used in gasket manufacturing. It includes the production of PVC, each plasticiser, and other additives present in the final gasket. As PVC and the additives are common to all six gaskets and not the focus of this analysis, they have been modelled using secondary data from Ecoinvent. While the synthesis of each plasticiser has been modelled in the foreground of the system using various data from literature sources.

Di-(2-ethyl hexyl) Phthalate – DEHP

Di-(2-ethyl hexyl) Phthalate (DEHP) is an organic compound, at room temperature appears as transparent liquid. From the structural point of view, it is the ester of the phthalic acid and two molecules of the 2-ethylhexanol.

The production of DEHP is done through an esterification process in two steps. The first is the reaction between the phthalic anhydride and the 2-ethylhexanol which gives the mono-ester and water as a by-product. This reaction is driven from its equilibrium to complete conversion of the reactants. The second reaction is the formation of the DEHP. In this case to push the equilibrium of this reaction towards the product, the water is separated between the steps and the second reactor use an excess of alcohol.

The reactor operates at medium (140-160°C) or high temperatures (200-250°C) depending on the chosen catalyst. After the second reaction step, the remaining alcohol is recovered through distillation and recirculated to the reactors (COWI et al., 2009).

The life cycle assessment (LCA) model for DEHP production was built using stoichiometric quantities of each reactant and data extracted from the Di-isononyl phthalate (DINP) ecoprofile (ECPI, 2015) as proxy for energy consumption and water balance. The quantity of catalyst used is typically a strong inorganic acid (as sulfuric acid) around 1 or 2% was considered below the cut-off threshold and therefore excluded from the analysis. The cut-off threshold, according to PEF method, is 3% on the single weighted score impact over the entire life cycle of the product.

Due to lack of information, stoichiometric quantities are used which do not account for reaction losses. Hence, for consistency reason all plasticiser models, will use the same assumption. This assumption seems also reasonable since the losses should be minimal due to the industrial maturity the processes involved (COWI et al., 2009).

The transport of raw materials was modelled using default distances for Europe as recommended by the PEF methodology, which are 270 km by truck, 240 km by train and 130 km by ship. This transport scenario is used consistently for all the plasticisers. Table 2 shows the input and output data for the DEHP production process, with the associated LCA dataset provide in the "Dataset" column. Unless otherwise specified, data from Ecoinvent was used.

The synthesis of the two precursors is described below, as they are part of the foreground system and of the life cycle of other plasticisers.

Table 2. Life cycle inventory to produce 1 kg of Di-(2-ethyl hexyl) Phthalate

Inventory data		Quantity	Unit	Dataset
Raw materials	Phthalic anhydride	0.379	kg	Phthalic anhydride {RER}| production | APOS, U
	2-ethyl hexanol	0.667	kg	Modelled as described in the 2-ethyl hexanol section
Transport	Ship	0.282	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.251	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.136	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U
Input	Heat	0.97	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Deionised water	0.14	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | APOS, U
	Cooling water	8.8	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
	Process water	0.004	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Output	Wastewater to WWTP	0.15	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U
	Water from cooling	8.5	kg	Water, Europe without Switzerland
	Water vapour	0.35	kg	-

Synthesis of phthalic anhydride

The production of phthalic anhydride follows two main pathways. The oldest and now less relevant is through the oxidation of naphthalene, the newest is the oxidation of ortho-xylene. The first process has declined in popularity in the last

decades due to the scarcity of the naphthalene as a by-product of the coke production (Lorz et al., 2007), while the xylene is a largely available. In the present study, due to its relevance, the production of phthalic anhydride from the oxidation of o-xylene route is used, using the ecoinvent dataset for the production of phthalic anhydride in Europe.

Synthesis of 2-ethyl hexanol

2-Ethyl hexanol is one of the most relevant alcohols produced globally. Largely used for the production of plasticisers, with a production volume of larger than 4 Mt per year (Agilent Research, 2022). The main industrial production process uses butyraldehyde as a feedstock. Another route using acetaldehyde is secondary due to its higher cost compared to butyraldehyde one. Butyraldehyde derives from oxo-synthesis, a refinery process involving the use of syngas to add a Carbon to an olefin such as propylene (Raff, 2013). The process happens in four steps:

1. Two butyraldehyde molecules condense in a reaction catalysed by a sodium hydroxide solution to produces ethyl hexanal and water. The ratio of butyraldehyde to aqueous solution varies in the range 1:10 - 1:20.
2. The alkaline solution and the organic phase spontaneously separate in a drum. After the separation, part of the aqueous solution is purged to eliminate the water produced in the reaction.
3. Then, the 2-ethyl-2-hexenal reaction is hydrogenated in a fixed catalyst bed reactors. The reaction is exothermic and heat may be used to produce steam.
4. The final product is separated from impurities through distillation (Bahrmann et al., 2013).

The two reactors do not require heating since they are both exothermic, the only part of the process that requires energy is the final purification of the alcohol, which was not possible to estimate it from literature, since it depends on the scale of the plant and its specific design choice (e.g. energy integration, use of steam ad different pressures).

This information was used to estimate the energy consumption for the separation. Energy integration was assumed to reuse of reaction heat into separation units, since it is a plausible practice for this reaction. In this case the heat released during the reaction is enough to cover the separation needs. Excess heat may be used in other parts of the plant, but to be conservative, no benefit from this energy were credited to the ethyl hexanol production. Water cooling was assumed with a net consumption of 5% of the circulating water, due to evaporation and losses, following the estimate made in Ecoinvent for similar industrial processes.

The quantity of reactants required per 1 kg of 2-ethylhexanol was calculated using stoichiometry of the reaction, assuming complete conversion of the

butyraldehyde at plant level, since the light co-products at the separated at the distillation column are reused into other processes such as the synthesis of butanol (Bahrmann et al.2013). The amount of sodium hydroxide to be replaced after step 2 is calculated considering a 2% concentration in the aqueous phase (Bahrmann et al., 2013).

The hydrogenation step is assumed to happen without losses of reagents since Bahrmann et al. (2013) report a 100% conversion and 99% selectivity achieved in this step. The consumption of catalyst is considered negligible and hence included in the cut-off, since heterogeneous catalyst have typically a very high reuse rate.

Table 3 shows the inputs and output of the unit process describing the production of 2-ethylhexanol.

Table 3. Life cycle inventory for the production of 1 kg of 2-ethyl hexanol

Inventory data		Quantity	Unit	Dataset
Input	Carbon monoxide	430	g	Carbon monoxide {RER}| production | APOS, U
	Hydrogen	62	g	Hydrogen, gaseous {Europe without Switzerland}| hydrogen production, gaseous, petroleum refinery operation | APOS, U
	Propylene	64.6	g	Propylene {RER}| production | APOS, U
	Sodium hydroxide	2.75	g	Sodium hydroxide, without water, in 50% solution state {RER}| chlor-alkali electrolysis, membrane cell | APOS, U
	Electricity	0.182	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
Output	Wastewater to treatment	0.138	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U

Acetyl tributyl citrate (ATBC)

ATBC is produced via a two-step reaction. In the first step, citric acid and butanol reacts, with help of acid catalyst (e.g. sulfuric acid), to produce Tributyl Citrate (TBC) (Osorio-Pascuas et al., 2015). The reaction proceeds at medium temperature (120°C) and 0.5–1.5% of catalyst concentration.

After, ATBC can be produced through direct esterification of TBC with acetic acid (Sakakura, Nakagawa, et al., 2007) or through acetylation with acetic anhydride (Sakakura, Kawajiri, et al., 2007). The latter synthesis route produces acetic acid as a by-product and it was selected to model the reaction.

Due to its low concentration and being inexpensive, the acetic acid produced typically is not recovered. In the inventory this flow does not appear since it was considered as part of the wastewater sent to treatment.

The stoichiometry was used to model the amount of each reagent for the plasticiser production. The raw materials' source is assumed to be in Europe, therefore the average distances prescribed in the PEF method (Annex I section 4.4.3.4) were applied. Table 4 summarises the amount of raw materials and transport required for the raw materials acquisition stage. Since no reliable data regarding the energy input for the ATBC manufacturing were found in literature, a process simulation software was used to estimate the energy flows. This approach relied on basic assumption for equipment design and should be considered as of lower quality than resorting to specific literature on industrial

processes. Below are briefly described the syntheses of acetic anhydride, citric acid and butanol.

Table 4. Life cycle inventory for the production of 1 kg of Acetyl tributyl citrate

Inventory data		Quantity	Unit	Dataset
Raw materials	Acetic Anhydride	0.254	kg	Acetic anhydride {RER}| production, ketene route | APOS, U
	Citric Acid	0.477	kg	Citric acid {RER}| production | APOS, U
	Butanol	0.552	kg	1-butanol {RER}| hydroformylation of propylene | APOS, U
Transport	Ship	0.347	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.308	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.167	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U
Input	Heat	0.462	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Cooling water	0.0048	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Output	Wastewater to WWTP	0.283	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U

Synthesis of acetic anhydride

The acetic anhydride is produced with the so-called ketene route, which starts with acetone being converted to methane and ketene, through its cracking at high temperature and pressure. In a second step the ketene reacts with acetic acid to form acetic anhydride while methane is burnt to provide part of the energy required by the process, while the other product, ketene, it further reacts with acetic acid to produce acetic anhydride (Held et al., 2000). The chemical was modelled using an Ecoinvent dataset as reported in Table 4.

Synthesis of citric acid

Citric acid is produced by a fermentation process, which employs the bacteria *Aspergillus niger* to convert sugars into citric acid. The dataset *Citric acid {RER}| production | APOS, U* from Ecoinvent was used to model it.

Synthesis of butanol

The industrial production of 1-butanol (also called n-butanol) is done by hydroformylation of propylene or from coal through a Fischer-Tropsch process (Hahn et al., 2013). In this study, it has been assumed that all the butanol is produced with the hydroformylation process to be more representative of the European production.

The production of all the ATBC precursors: citric acid, n-butanol and acetic anhydride is modelled with secondary data from Ecoinvent as shown in Table 4.

Di(2-ethyl hexyl) Adipate – DEHA

DEHA is one of the esters derived from adipic acid. It is used in various applications, from food packaging to construction sector. Its production is based on acid-catalysed esterification of adipic acid with 2-ethyl hexanol.

Primary data for the synthesis of the plasticiser were not available, therefore data from the ecoprofile of DINP (ECPI, 2015) were used as proxy for the DEHA since they both involve the esterification of a primary alcohol of similar weight a carboxylic acid or anhydride in liquid phase. The amount of catalyst consumed per unit of product is included in the cut-off.

The modelling of the plasticiser production has been developed using the stoichiometry to calculate the amount of adipic acid and 2-ethylhexanol needed. The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method have been assumed. Table 5 summarises the quantity of raw materials energy, auxiliary flows and transport required for the plasticiser manufacturing. The inputs and outputs to the manufacturing stage are modelled according to the DINP Ecoprofile.

Table 5. Life Cycle Inventory for the production of 1 kg of Di(2-ethyl hexyl) Adipate

Inventory data		Quantity	Unit	Dataset
Raw materials	Adipic acid	0.394	kg	Adipic acid {RER}| production | APOS, U
	2-ethylhexanol	0.703	kg	See Table 3
Energy and auxiliary input	Heat	0.97	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Deionised water	0.14	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | APOS, U
	Cooling water	8.8	l	Water, cooling, unspecified natural origin, Europe without Switzerland
	Process water	0.004	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Waste and output	Wastewater to WWTP	0.15	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U
	Water from cooling	8.5	kg	Water, Europe without Switzerland
	Water	0.35	kg	-
Transport	Ship	0.296	tkm	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.263	tkm	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.143	tkm	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Synthesis of Adipic Acid

Adipic acid, it is a basic chemical for the synthesis of a wide range of molecules (Skoog et al., 2018) but about the 65% of the global production is used to produce nylon-6,6-polyamide (Deng & Mao, 2015); it is also used to produce polyurethanes, paints, coatings, plasticisers and as food additive (Polen et al., 2013). Its production process is based on the oxidation of a mixture of cyclohexanol and cyclohexanone with nitric acid. This mixture is the result of the oxidation of cyclohexane. The production of adipic acid in this study is modelled with secondary data from Ecoinvent, while the supply chain of the ethyl hexanol is described in Table 3.

Di(2-ethyl hexyl) Terephthalate - DEHT

The DEHT is produced by the esterification of terephthalic acid and 2-ethylhexanol. Terephthalates are sometimes used as alternative to the corresponding phthalate in some applications since they have a similar chemical structure and similar technical properties.

The modelling of the input for the plasticiser production has been developed using the stoichiometry to calculate the amount of terephthalic acid and 2-ethylhexanol. The catalyst used to promote the esterification is included in the cut-off, as for the other plasticisers. The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method have been assumed. Table 6 summarise the quantity of raw materials, energy, auxiliary flows and transport required for the raw material acquisition stage.

Table 6. Life Cycle Inventory for the production of 1 kg of Di(2-ethyl hexyl) terephthalate

Inventory data		Quantity	Unit	Dataset
Raw materials	Terephthalic acid	0.425		Purified terephthalic acid {RER}| production | APOS, U
	2-ethylhexanol	0.667	kg	See Table 3
Energy and auxiliary input	Heat	0.97	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Deionised water	0.14	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | APOS, U
	Cooling water	8.8	l	Water, cooling, unspecified natural origin, Europe without Switzerland
	Process water	0.004	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Waste and output	Wastewater to WWTP	0.15	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U
	Water from cooling	8.5	kg	Water, Europe without Switzerland
	Water	0.35	kg	-
Transport	Ship	0.295	tkm	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.262	tkm	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.142	tkm	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Synthesis of terephthalic acid

Terephthalic acid is one of the most relevant chemical since it is used for the synthesis of polyethylene terephthalate (PET). The industrial production is done starting from p-xylene coming from BTX fractionation, using almost completely the Amoco process. Given the high purity standards required for PET production, the primary application of terephthalic acid, the manufacturing process includes a purification stage. This involves hydrogenating impurities followed by distillation to remove residual p-xylene and other by-products that can affect the final product's color (J. Sheehan, 2011). The production of terephthalic acid is modelled with secondary data from ecoinvent.

Di-isononyl cyclohexanoate – DINCH

Cyclohexanoates are plasticisers derived from the phthalates through the hydrogenation of the aromatic ring. Owing to their structural similarity to phthalates, they can serve as direct substitutes while mitigating associated safety concerns. One of the most widely used cyclohexanoates is DINCH, produced via the catalytic hydrogenation of DINP. Although detailed process data are not publicly disclosed, the synthesis pathway can be partially reconstructed from patents (Brunner et al., 2001) and by analogies with other hydrogenation processes, such as the hydrogenation of benzene to cyclohexane, using Ecoinvent datasets.

The production route for DINP and its precursors closely resembles that of DEHP. Isononyl alcohol, a key intermediate, is synthesized via the hydroformylation of alkenes with 8 Carbon atoms (C8), which may originate from dimerisation of n-butene separated by the C4 raffinate, or alternatively via the polygas process, using the same C4 feedstock but yielding a mixture of C7–C9 alkanes. The isononyl alcohol subsequently reacts with phthalic anhydride to form DINP. In the present study, the LCA of DINCH is modelled based on existing LCI data for DINP, as reported by European Plasticisers. (ECPI, 2015).

The unit process for the raw material acquisition of the plasticiser is created using secondary data for the precursors (DINP and hydrogen). The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method have been assumed. The inputs and outputs required for the hydrogenation process are unknown, hence proxy data were extracted from the hydrogenation of benzene to cyclohexane using the Ecoinvent dataset *Cyclohexane {RER}| production | APOS, U*. The quantity of the raw materials, transport, energy and auxiliary materials required for the plasticiser manufacturing are summarised in Table 7 shows a summary of the unit process inputs and outputs.

Table 7. Life Cycle Inventory for the production of 1 kg of Di-isononyl cyclohexanoate

Inventory data		Quantity	Unit	Dataset
Raw materials	DINP	0.986	kg	Dataset derived from DINP Ecoprofile
	Hydrogen	0.014	kg	Hydrogen, gaseous {Europe without Switzerland}| hydrogen production, gaseous, petroleum refinery operation | APOS, U
Energy and auxiliary input	Heat	2.82	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Heat	1.57	MJ	Heat, district or industrial, other than natural gas {RER}| market group for | APOS, U
	Electricity	0.127	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
	Catalyst	0.03	g	Nickel 99.5% {GLO}| market for | APOS
	Deionised water	0.95	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | APOS, U
	Cooling water	8.8	l	Water, cooling, unspecified natural origin, RER[1]
	Water	0.35	kg	-
Transport	Ship	0.270	tkm	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.240	tkm	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.130	tkm	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

[1] This flow of water is modelled with an elementary flow, directly released into the environment.

Epoxidised soybean oil (ESBO)

ESBO production process involves soybean oil, an aqueous solution containing hydrogen peroxide (H_2O_2) and formic or acetic acid and sulfuric or phosphoric acid (Alhanish & Abu Ghalia, 2021). The organic acid reacts with hydrogen peroxide to form a peroxy acid, which can diffuse into the oil and epoxidise it. This reaction regenerates the initial organic acid which then acts similarly to a catalyst. The reaction, normally, requires 6-10 hours to be completed keeping the temperature between 60 and 75°C.

The production of soybean oil and hydrogen peroxide is modelled using secondary data from Ecoinvent. The formic and sulphuric acid used are considered in the cut-off, since they act as catalyst in the reaction. The energy requirements in the epoxidation process, the water consumption and the waste produced come from the information disclosed in an Environmental Product Declaration published by an ESBO manufacturer (Hairma (Nantong) Technology, 2022). Table 8 summarises the before mentioned inventory flows. A short description of the production route of the raw materials is provided below.

Table 8. Life cycle inventory for the production of 1 kg of Epoxidised soybean oil

Inventory data		Quantity	Unit	Dataset
Raw materials	Soybean oil	0.902	kg	Soybean oil, crude {RER}| soybean meal and crude oil production | APOS, U
	Hydrogen peroxide	0.209	kg	Hydrogen peroxide, without water, in 50% solution state {RER}| market for hydrogen peroxide, without water, in 50% solution state | APOS, U
Energy and auxiliary input	Steam	0.143	MJ	Steam, in chemical industry {RER}| production | APOS, U
	Electricity	0.0371	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
	Water	0.0002	kg	Water, river, Europe without Switzerland
Waste and emission	Hazardous waste	0.0013	kg	Refinery sludge {Europe without Switzerland}| treatment of refinery sludge, hazardous waste incineration | APOS, U
Transport	Ship	0.300	tkm	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.267	tkm	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.144	tkm	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Extraction of soy oil

Soybean oil is extracted from soybeans through a process involving several steps. First, the soybeans are cleaned, dehulled, and cracked to break them into smaller pieces. The cracked beans are then heated to ease oil extraction. Mechanical pressing or solvent extraction methods are typically used to extract the oil. In mechanical pressing, the soybeans are pressed to release the oil, while in solvent extraction, a solvent like hexane is used to extract the oil (Riaz, 2005). The production of soy oil was modelled using a dataset from Ecoinvent, as reported in Table 8.

Synthesis of Hydrogen Peroxide

The most common process for the production of hydrogen peroxide is the auto-oxidation (AO) or anthraquinone process, which is the most relevant

industrial process nowadays. In a first step, hydrogen peroxide is produced by reducing alkyl-anthraquinone with hydrogen with a metal catalyst (e.g. Palladium) to the corresponding anthra-hydroquinone. Then the catalyst is removed and the hydroquinone is oxidised back to the quinone producing a molecule of hydrogen peroxide (Goor et al., 2019). The production of hydrogen peroxide was modelled using a dataset from Ecoinvent, as reported in Table 8.

PVC and additives

For the modelling of the PVC that is blended with the plasticiser, a secondary dataset representative of emulsion PVC, since this is the polymer commonly used for the plastisol applications. Other additives are also modelled using secondary datasets from Ecoinvent as shown in Table 9. This limitation is due to data availability but it is acceptable considering that the purpose of the study is to evaluate differences in impacts of different plasticisers. Since no secondary dataset for zinc stearate production is available, a customized dataset was created with literature data. Zinc stearate is produced heating zinc oxide and stearic acid at 140 °C and at atmospheric pressure (Gönen et al., 2005). Table 9 shows the inputs and output calculated using stoichiometry calculations. Energy consumption for heating or cooling is assumed to be negligible and considered a cut-off, since the amount of Zinc stearate used in the final product is around 1% in mass.

Table 9. Life cycle inventory for the production of 1 kg of Zinc stearate

Inventory data		Quantity	Unit	Dataset
Input	Zinc Oxide	0.130	kg	Zinc oxide {RER}| production | APOS, U
	Stearic Acid	0.9	kg	Stearic acid {GLO}| stearic acid production | APOS, U
Output	Water	0.0285	l	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U

1.2.2 Compounding and manufacturing of the gasket

This section reports the modelling and inventory for the production of the gasket. This activity includes the production of the plastisol and the production of the gasket that is applied inside the metal lid. These two processes are often done in the same facility, since the metal cap producer is usually producing its own plastisol, hence no transport between the two processes was considered.

Plastisol Production and gasket manufacturing

The inventories of plastisol production for each plasticiser are reported. The composition reported in Table 10 is based on Bayer et al., (1988); Giessler & Ratliff, (1968) and confirmed by industrial stakeholders.

Below, Table 10 shows the energy and utilities requirements for mixing and cooling the compound. The energy requirements were estimated from a previous

work, in which a similar mixture was applied (Boluk et al., 1990), while the cooling water was calculated based on the experimental study of Nakajima (2000) assuming a net loss of 5% in the industrial application. The amount of energy and cooling water consumption was assumed to be independent from the plasticiser choice.

Finally, the plastisol is molded into the metal lid and then cured passing through an oven (Graham, 1973). In this step, the PVC particles and the plasticiser melt together to form a homogeneous material with the desired mechanical properties once it is cooled (Marcilla et al., 2017). Temperature for curing ranges from 150°C to 190°C (Graham, 1973). The energy requirement for this process has been estimated from a study in which a similar PVC compound is cured in a high-velocity hot-air tunnel oven (Boluk et al., 1990). Table 11 shows the energy requirements for the processes described in this section.

Table 10. Life cycle inventory for the production of 1 kg of plastisol, for each type of gasket

Data inventory		DEHP	ATBC	DEHA	DEHT	DINCH	ESBO	Unit	Dataset
Input	Plasticiser	358.2	371.7	341.7	365.0	378.2	394.0	g	See Section 1.2.1
	E-PVC	477.6	467.5	489.8	472.5	462.6	456.7	g	Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation | APOS, U
	Blowing Agent (Sodium Bicarbonate)	5.73	5.6	5.9	5.7	5.6	5.21	g	Sodium bicarbonate {RER}| soda production, solvay process | APOS, U
	Stabiliser (Zinc Stearate)	11.94	11.7	12.2	11.8	11.6	10.85	g	See Table 9
	Lubricant (stearic acid)	40.59	39.7	41.6	40.2	39.3	36.90	g	Stearic acid {GLO}| stearic acid production | APOS, U
	Pigment (TiO2)	5.731	5.6	5.9	5.7	5.6	5.210	g	Titanium dioxide {RER}| production, sulfate process | APOS, U
	Filler (calcium carbonate)	100.3	98.2	102.9	99.2	97.2	91.2	g	Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated | APOS, U
Energy	Electricity	0.917						kWh	Electricity, medium voltage {RER}| market group for | APOS, U
Auxiliary	Cooling water	0.0565						m^3	Water, cooling, unspecified natural origin, RER
Transport	Ship	0.270	0.270	0.270	0.270	0.270	0.270	tkm	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.240	0.240	0.240	0.240	0.240	0.240	tkm	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.130	0.130	0.130	0.130	0.130	0.130	tkm	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Table 11. Life cycle inventory for the production of 1 kg of gaskets

Input	Quantity	Unit	Dataset
Heat for pre-heating	0.108	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
Electricity for curing	0.883	kWh	Electricity, medium voltage {RER}| market group for | APOS, U

1.2.3 Distribution

The distribution phase considers the transport of the gasket is used to the final customer, which is the company using it as food packaging. Even if the physically the cap and its gasket are joined and transported together, the freight transport is allocated to each of them based on their mass. Therefore, only the mass of the gasket is considered in the system boundaries of the study. Due to the foreseeable small contribution of this phase to the final results, the average transport scenario for the packaging material from PEF method is used as presented in Table 12.

Table 12. Inventory flows for the transport of 1 kg of gaskets

Mode of transport	Quantity	Unit	Dataset
Ship	0.360	tkm	Transport, freight, inland waterways, barge {RER}| market| APOS, U
Train	0.280	tkm	Transport, freight train {Europe without Switzerland}| market for | APOS, U
Truck	0.230	tkm	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

1.2.4 Use phase

The use phase of the gasket begins when the cap is used in the canning process. In this phase no input or output flow can be directly attributed directly to the gasket and any process (transport, refrigeration, labelling etc.) involved in this phase is done for the purpose of preserving the food, and therefore the environmental impact shall be accounted in the system boundaries of the food and excluded from the gasket boundaries. The final use of the gasket is linked to the use of the cap, the jar and its content. Since it is used as food packaging it can be assumed to be a single use packaging. Therefore, no relevant input in this phase of the life cycle contributes to the final impacts of the gasket.

1.2.5 End-of-life

The share of waste caps sent to incineration or disposal has been assumed using the data of the average European municipal waste treatment (Eurostat, 2022), which is 53% to incineration and 47% to landfill. Following this scenario, the materials composing the gasket (PVC, plasticiser and additives) were distributed to the two disposal scenarios, proportionally to their mass, as depicted in Figure 3.

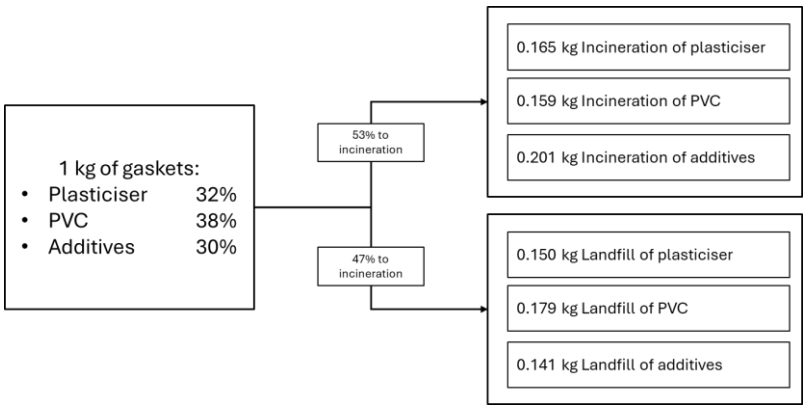

Figure 3. Waste management model of the gasket disposal, with the share of each disposal scenario

The disposal of each component of the gasket is modelled specifically considering its elementary composition (see Table 13).

For each plasticiser a unit process for the incineration and one for the sanitary landfill have been developed, which model the specific emissions due to either the incineration or landfill of each plasticiser. This was done using the model developed in Doka (2020), fed with the elementary composition of the plasticisers. Then, the plasticiser specific dataset was coupled with the equivalent dataset for the disposal of PVC from Ecoinvent and with the one developed for the disposal of the additives.

Finally, the inventory of the end-of-life of the whole gasket is modelled using the described dataset aggregated considering the share of each material (PVC, plasticiser and additives) and the share of treatment as shown in Table 14. A summary of the life cycle inventory per each type of gasket is provided in Table 15 and Table 16 showing the inputs and outputs of the customized dataset developed for the incineration and landfill respectively.

Table 13. Elementary composition of each gasket of each gasket based on the plasticiser used

Elementary composition	**DEHP [%]**	**ATBC [%]**	**DEHA [%]**	**DEHT [%]**	**DINCH [%]**	**ESBO [%]**	**Additives [%]**
C	73.8	59.7	71.3	73.8	74.2	70.2	33.0
H	9.8	8.5	11.4	9.8	10.5	10.1	4.3
O	16.4	31.8	17.3	16.4	15.2	19.7	35.3
Na	0	0	0	0	0	0	0.8
Ca	0	0	0	0	0	0	24.8
Zn	0	0	0	0	0	0	0.9
Ti	0	0	0	0	0	0	1.7
% of biogenic C	0	30	0	0	0	100	34

Table 14. Summary of the waste management for 1 kg of each gasket

Input	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO	Unit	Dataset
Incineration of plasticiser	0.190	0.197	0.181	0.193	0.200	0.201	kg	Custom dataset (see Table 15)
Incineration of the PVC	0.253	0.248	0.260	0.250	0.245	0.244	kg	Waste polyvinylchloride {CH}| treatment of, municipal incineration | APOS, U
Incineration of additives	0.087	0.085	0.089	0.086	0.084	0.084	kg	Custom dataset (see Table 15)
Landfill of plasticiser	0.168	0.175	0.161	0.172	0.178	0.179	kg	Custom dataset (see Table 16)
Landfill of the PVC	0.225	0.220	0.230	0.222	0.217	0.217	kg	Waste polyvinylchloride {CH}| treatment of, sanitary landfill | APOS, U
Landfill of additives	0.077	0.076	0.079	0.076	0.075	0.075	kg	Custom dataset (see Table 16)

Table 15. Life cycle inventory for the incineration of 1 kg of each plasticiser and additives

	Unit	DEHP	ATBC	DEHA	DINCH	DEHT	ESBO	Additives	Dataset
Metalliferous hydroxide sludge	kg	4.6E-04	3.7E-04	4.5E-04	4.6E-04	4.6E-04	4.4E-04	2.2E-02	Metalliferous hydroxide sludge {GLO}| market for metalliferous hydroxide sludge | APOS, U
Sodium hydroxide, without water, in 50% solution	kg	2.5E-05	2.0E-05	2.4E-05	2.5E-05	2.5E-05	2.4E-05	1.2E-03	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, U
Hydrochloric acid, without water, in 30% solution	kg	3.9E-05	3.1E-05	3.7E-05	3.9E-05	3.9E-05	3.7E-05	1.6E-03	Hydrochloric acid, without water, in 30% solution state {RER}| market for | APOS, U
Inorganic chemicals	kg	1.8E-05	1.4E-05	1.7E-05	1.8E-05	1.8E-05	1.7E-05	1.1E-04	Chemical, inorganic {GLO}| market for chemicals, inorganic | APOS, U
Cement	kg	7.2E-04	5.8E-04	6.9E-04	7.2E-04	7.2E-04	6.8E-04	2.3E-02	Cement, unspecified {CH}| market for cement, unspecified | APOS, U
Waste cement, hydrated	kg	1.8E-03	1.5E-03	1.7E-03	1.8E-03	1.8E-03	1.7E-03	5.8E-02	Waste cement, hydrated {CH}| market for waste cement, hydrated | APOS, U
Transport, freight, lorry	t*km	6.5E-04	5.6E-04	6.3E-04	6.5E-04	6.5E-04	6.2E-04	1.9E-02	Transport, freight, lorry 16-32 metric ton, EURO4 {RER}| transport, freight, lorry 16-32 metric ton, EURO4 | APOS, U
Ammonia, liquid	kg	8.3E-04	6.3E-04	8.5E-04	8.6E-04	8.3E-04	8.0E-04	3.15E-04	Ammonia, liquid {RER}| market for | APOS, U
Heat, district or industrial, natural gas	MJ	1.6E-01	1.2E-01	1.6E-01	1.6E-01	1.6E-01	1.5E-01	5.9E-02	Heat, district or industrial, natural gas {CH}| market for heat, district or industrial, natural gas | APOS, U
Titanium dioxide	kg	5.2E-05	3.9E-05	5.3E-05	5.4E-05	5.2E-05	5.0E-05	2.0E-04	Titanium dioxide {RER}| market for | APOS, U
Chromium oxide, flakes	kg	1.1E-06	8.0E-07	1.1E-06	1.1E-06	1.1E-06	1.0E-06	4.03E-07	Chromium oxide, flakes {GLO}| market for | APOS, U
Hydrogen peroxide, without water, 50% solution	kg	8.7E-05	7.0E-05	8.4E-05	8.7E-05	8.7E-05	8.3E-05	4.1E-03	Hydrogen peroxide, without water, in 50% solution state {RER}| market for hydrogen peroxide, without water, in 50% solution state | APOS, U
Spent activated carbon with mercury	kg	1.8E-05	1.4E-05	1.7E-05	1.8E-05	1.8E-05	1.7E-05	1.1E-04	Spent activated carbon with mercury {GLO}| market for | APOS, U
Water, decarbonised	kg	2.1E-01	1.7E-01	2.0E-01	2.1E-01	2.1E-01	2.0E-01	1.3E+00	Water, decarbonised {CH}| water production, decarbonised | APOS, U
Municipal waste incineration facility	unit	2.5E-10	2.5E-10	2.5E-10	2.5E-10	2.5E-10	2.5E-10	2.5E-10	Municipal waste incineration facility {CH}| construction | APOS, U
Slag landfill	unit	2.4E-11	2.1E-11	2.4E-11	2.4E-11	2.4E-11	2.4E-11	7.1E-10	Slag landfill {CH}| construction | APOS, U
Process-specific burdens, slag landfill	kg	1.4E-02	1.2E-02	1.3E-02	1.4E-02	1.4E-02	1.3E-02	4.0E-01	Process-specific burdens, slag landfill {CH}| processing | APOS, U
Residual material landfill	unit	3.7E-12	3.0E-12	3.6E-12	3.8E-12	3.7E-12	3.6E-12	1.2E-10	Residual material landfill {CH}| construction | APOS, U
Process-specific burdens, residual material landfill	kg	1.8E-03	1.5E-03	1.7E-03	1.8E-03	1.8E-03	1.7E-03	5.7E-02	Process-specific burdens, residual material landfill {CH}| processing | APOS, U
Input from nature									

Oxygen, from air	kg	5.2E+00	3.9E+00	5.3E+00	5.3E+00	5.2E+00	5.0E+00	1.96E+00	
Emissions to air									
Carbon monoxide, fossil	kg	2.4E-05	1.1E-05	2.2E-05	2.2E-05	2.4E-05		4.9E-05	
Carbon monoxide, biogenic	kg		2.7E-05				2.6E-05	1.3E-05	
Carbon dioxide, fossil	kg	2.7E+00	6.5E-01	2.6E+00	2.7E+00	2.7E+00		9.5E-01	
Carbon dioxide, biogenic	kg		1.5E+00				2.6E+00	2.5E-01	
Methane, fossil	kg	2.1E-07	1.0E-07	1.9E-07	1.9E-07	2.1E-07		4.3E-07	
Methane, biogenic	kg		2.4E-07				2.3E-07	1.1E-07	
Nitrogen oxides	kg	3.1E-04	2.3E-04	3.2E-04	3.2E-04	3.1E-04	3.0E-04	1.17E-03	
Ammonia	kg	9.8E-07	7.4E-07	1.0E-06	1.0E-06	9.8E-07	9.4E-07	3.7E-07	
NMVOC, non-methane volatile organic compounds	kg	6.3E-07	1.0E-06	5.9E-07	5.8E-07	6.3E-07	6.9E-07	1.65E-06	
Particulates, < 2.5 um	kg	1.7E-06	2.7E-06	1.5E-06	1.5E-06	1.7E-06	1.8E-06	4.3E-06	
Particulates, > 2.5 um, and < 10um	kg	8.3E-09	1.3E-08	7.8E-09	7.6E-09	8.3E-09	9.1E-09	2.2E-08	
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin	kg	2.8E-14	4.5E-14	2.6E-14	2.5E-14	2.8E-14	3.0E-14	7.2E-14	
Benzene	kg	1.4E-08	2.2E-08	1.3E-08	1.3E-08	1.4E-08	1.5E-08	3.6E-08	
Toluene	kg	2.8E-08	4.5E-08	2.6E-08	2.5E-08	2.8E-08	3.0E-08	7.2E-08	
Benzene, pentachloro-	kg	7.3E-11	1.2E-10	6.8E-11	6.7E-11	7.3E-11	8.0E-11	2.0E-10	
Benzene, hexachloro-	kg	2.9E-11	4.7E-11	2.7E-11	2.7E-11	2.9E-11	3.2E-11	7.6E-11	
Phenol, pentachloro-	kg	6.0E-12	9.8E-12	5.6E-12	5.5E-12	6.0E-12	6.6E-12	1.6E-11	
Benzo(a)pyrene	kg	3.1E-13	5.0E-13	2.9E-13	2.8E-13	3.1E-13	3.4E-13	8.1E-13	
Water	m3	9.2E-04	7.9E-04	1.0E-03	9.8E-04	9.2E-04	9.4E-04	1.1E-03	
Emissions to water									
Water	m3	7.1E-05	5.7E-05	6.9E-05	7.2E-05	7.1E-05	6.8E-05	4.2E-03	
BOD5, Biological Oxygen Demand	kg	5.5E-04	4.4E-04	5.3E-04	5.5E-04	5.5E-04	5.2E-04	2.5E-04	
COD, Chemical Oxygen Demand	kg	5.6E-04	4.5E-04	5.4E-04	5.6E-04	5.6E-04	5.3E-04	2.5E-04	
TOC, Total Organic Carbon	kg	2.4E-04	2.0E-04	2.4E-04	2.5E-04	2.4E-04	2.3E-04	1.1E-04	
DOC, Dissolved Organic Carbon	kg	2.4E-04	2.0E-04	2.4E-04	2.5E-04	2.4E-04	2.3E-04	1.1E-04	

BOD5, Biological Oxygen Demand, long-term	kg	1.8E-03	1.4E-03	1.7E-03	1.8E-03	1.8E-03	1.7E-03	2.5E-04	
COD, Chemical Oxygen Demand, long-term	kg	5.5E-03	4.4E-03	5.3E-03	5.5E-03	5.5E-03	5.2E-03	2.5E-04	
TOC, Total Organic Carbon, long-term	kg	2.2E-03	1.8E-03	2.1E-03	2.2E-03	2.2E-03	2.1E-03	1.1E-04	
DOC, Dissolved Organic Carbon, long-term	kg	2.2E-03	1.8E-03	2.1E-03	2.2E-03	2.2E-03	2.1E-03	1.1E-04	

Table 16. Life cycle inventory for the disposal of 1 kg of each plasticiser and additives in landfill

	Unit	**DEHP**	**ATBC**	**DEHA**	**DINCH**	**DEHT**	**ESBO**	**Additives**	**Dataset**
Transport, freight, lorry	t*km	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	Transport, freight, lorry >32 metric ton, EURO4 {RER}| transport, freight, lorry >32 metric ton, EURO4 | APOS, U
Heat, district or industrial, natural gas	MJ	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	Heat, district or industrial, natural gas {RER}| market group for | APOS, U
Electricity, low voltage	kWh	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	Electricity, low voltage {RER}| market group for | APOS, U
Heat, district or industrial, other than natural gas	MJ	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	Heat, district or industrial, other than natural gas {Europe without Switzerland}| market for heat, district or industrial, other than natural gas | APOS, U
excavation, hydraulic digger	m3	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	Excavation, hydraulic digger {RER}| processing | APOS, U
excavation, skid-steer loader	m3	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	Excavation, skid-steer loader {RER}| processing | APOS, U
diesel, burned in building machine	MJ	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	Diesel, burned in building machine {GLO}| market for | APOS, U
gravel, round	kg	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	Gravel, round {CH}| gravel and sand quarry operation | APOS, U
tap water	kg	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	Tap water {Europe without Switzerland}| tap water production, conventional with biological treatment | APOS, U
Input from nature									
Occupation, construction site	m2*y	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	
Occupation, dump site	m2*y	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	
Occupation, shrub land, sclerophyllous	m2*y	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	

Occupation, traffic area, road network	m2*y	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	
Transformation, from pasture, man made	m2	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	
Transformation, from dump site, sanitary landfill	m2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, from shrub land, sclerophyllous	m2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to dump site, sanitary landfill	m2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to shrub land, sclerophyllous	m2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to forest, unspecified	m2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to traffic area, road network	m2	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	
Input from nature									
Oxygen, from air	kg	5.2E+00	3.9E+00	5.3E+00	5.3E+00	5.2E+00	5.0E+00	1.96E+00	
Emissions to water									
BOD5, Biological Oxygen Demand, long term	kg	0.191	0.155	0.185	0.193	0.192	0.191	0.182	
COD, Chemical Oxygen Demand, long term	kg	0.807	0.653	0.780	0.816	0.812	0.807	0.768	
TOC, Total Organic Carbon, long term	kg	0.738	0.597	0.713	0.746	0.742	0.738	0.702	
DOC, Dissolved Organic Carbon	kg	0.738	0.597	0.713	0.746	0.742	0.738	0.702	

1.3 Life Cycle Impact Assessment

LCA impacts at the midpoint are calculated using the Environmental Footprint impact assessment method (version 3.1). This method was selected due to its comprehensive coverage of sixteen impact categories, encompassing all the relevant aspects of the framework, and since it 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 non-cancer). These categories address potential safety concerns arising from the indirect exposure (i.e. exposure due to the presence in the environment of the chemical rather than due to the interaction of the target with the source of the chemical) 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).

Following the PEF method, the potential environmental impacts are calculated at the midpoint characterisation level for the life cycle of each of the six different plasticized gaskets (see Table 17).

Table 17. Summary of the midpoint results of the LCIA of the six gaskets

Impact Category	Unit	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Human toxicity, cancer	CTUh	1.93E-09	2.28E-09	3.21E-09	1.90E-09	1.66E-09	2.65E-09
Human toxicity, non-cancer	CTUh	3.84E-08	5.03E-08	4.18E-08	3.83E-08	3.43E-08	3.77E-08
Ecotoxicity, freshwater	CTUe	5.78E+01	7.03E+01	6.02E+01	5.72E+01	5.45E+01	6.13E+01
Climate change	kg CO_2 eq	4.19E+00	4.51E+00	5.71E+00	4.14E+00	4.34E+00	5.51E+00
Ozone depletion	kg CFC11 eq	9.07E-07	9.74E-07	9.75E-07	9.05E-07	7.98E-07	8.06E-07
Particulate matter	Disease inc	1.18E-07	1.45E-07	1.43E-07	1.06E-07	1.01E-07	1.06E-07
Ionising radiation	kBq U_{235} eq	7.76E-01	8.45E-01	7.81E-01	7.72E-01	8.18E-01	6.87E-01
Photochemical ozone formation	kg NMVOC eq	9.94E-03	1.13E-02	1.08E-02	9.11E-03	9.12E-03	9.03E-03
Acidification	mol H^+ eq	1.72E-02	2.19E-02	1.95E-02	1.65E-02	1.59E-02	1.55E-02
Eutrophication, terrestrial	molc N eq	3.52E-02	4.94E-02	4.10E-02	3.45E-02	3.36E-02	3.63E-02
Eutrophication, freshwater	kg P eq	1.56E-03	1.83E-03	1.68E-03	1.55E-03	1.39E-03	1.59E-03
Eutrophication, marine	kg N eq	3.36E-03	4.75E-03	3.71E-03	3.27E-03	3.16E-03	8.27E-03
Water use	m^3 water eq	5.18E+00	7.72E+00	5.29E+00	5.14E+00	5.28E+00	5.16E+00
Land use	Pt	1.06E+02	8.09E+02	1.14E+02	1.04E+02	9.92E+01	4.52E+02
Resource use, fossil	MJ	8.73E+01	8.93E+01	9.25E+01	8.55E+01	8.92E+01	6.03E+01
Resource use, minerals and metals	kg Sb eq	4.69E-05	6.55E-05	5.21E-05	4.85E-05	4.08E-05	5.26E-05

The midpoint results are compared to the results of the reference gasket (the one containing DEHP). To do so, the percentage change of the impact for the five plasticiser compared to the DEHP one is calculated and showed in Table 18.

Table 18. Percentage change of the environmental impact of the five alternative gaskets compared to the reference one

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

The characterised results are also normalised and weighted using the factors recommended by the PEF. The normalisation and weighting process is used in PEF to compute a final single score that can aggregate all the impact categories (see Figure 5).

The PEF method includes a set of weighing factors developed with the contribution of domain experts as well as reflecting panel-based elicitations, aiming to reflect the relevance and the scientific robustness of the different impact categories (Sala et al., 2018) and these results. Since these factors were developed in another context, they were used for the case study as a test but not adopted as an aggregation method of the different impact categories in SSbD framework.

The results across the impact categories show two different patterns. Some impact categories do not show significant differences among the plasticisers, such as the “Ionizing radiation, human health” and “Ecotoxicity, freshwater”, while others show significant differences among some of them, such as the “resource use, fossils” and the “land use”. Similarities and differences can be attributed mostly to the type and quantity of the plasticiser since the quantity of PVC and the additives change according to the plasticiser substitution factor. In most cases, the precursors are petrochemicals, except for the ESBO and partly for the ATBC that are bio-based (i.e. the soy oil and the citric acid, respectively). This is reflected, for example, in the “land use” impact category for ATBC and ESBO which is higher than for all the other plasticisers due their precursors (+665% and +327% respectively), while ESBO scores lower than all the others on the “resource use, fossil” (-31%). Regarding the climate change indicator, DEHA shows the highest results, due to the higher impact of its raw materials, followed by ESBO due to the emissions linked to land use change in soy oil production. In Figure 4, a breakdown of the climate change impacts is shown for the life cycle stages of each gasket. It can be seen that the raw material acquisition (i.e. the impacts

related to the production of the precursors for each plasticiser) accounts for at least half of the impacts in all the cases, accounting for most of the difference on the final result.

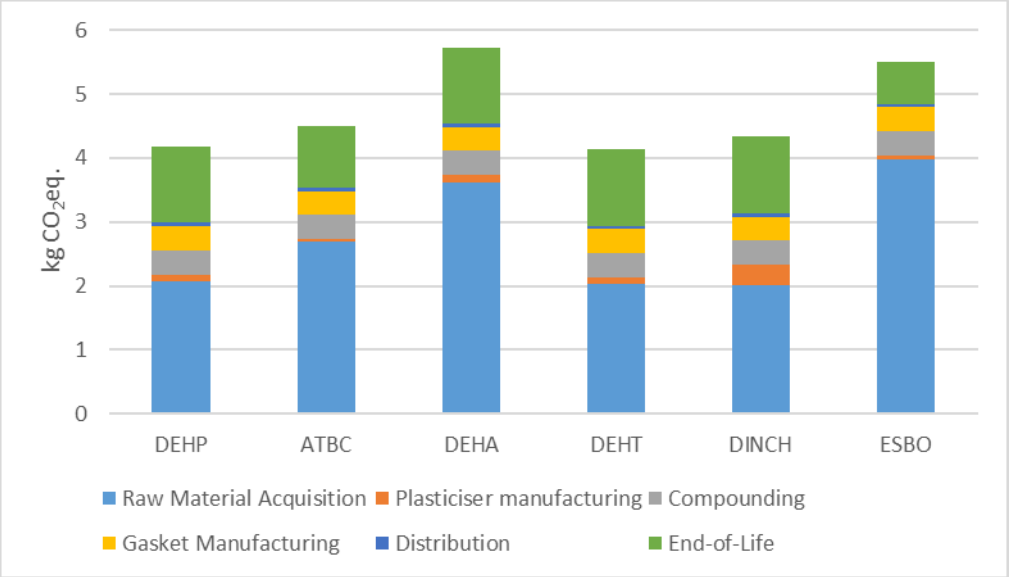

Figure 4. Climate change impacts for the six gaskets, divided by life cycle stage.

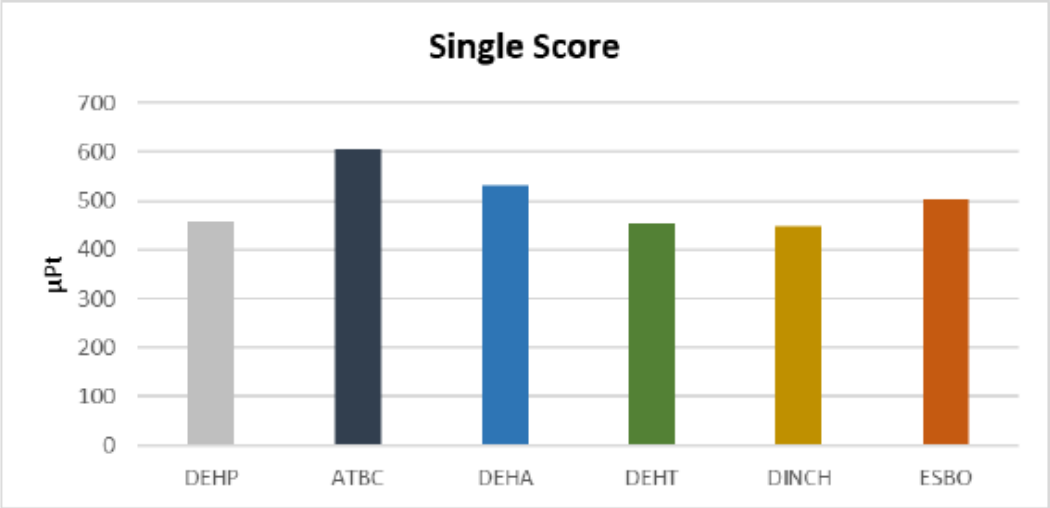

Figure 5. Single weighted score for the six gaskets. Calculated using the Product Environmental Footprint recommended Normalisation and weighting sets

1.4 Challenges

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

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, and therefore a benchmark is needed for each impact category. The most common way to address this aspect in 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 users and can substitute each other, making them comparable. This is explicitly required both by the ISO 14040 and 14044 standards and by the PEF methodology. PEF, in addition, define benchmarks 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 one of the principles used to define benchmarks in the PEF method.

In the case study, the environmental impacts of each gasket are compared to the DEHP gasket, that have been chosen as a reference, since it is a general-purpose plasticiser, 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 and the method used to calculate the composition of the different gaskets described in previous sections. The study simulates the case in which a company wants to find an alternative to an existing chemical.

In both cases, these approaches allow to measure 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 lead 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. A tentative 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.

Then it is important for the application of the SSbD framework that a benchmark 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

LCA 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 into 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).

The goal of the SSbD framework includes the ability to compare alternative chemicals also at intermediate level and the definition of a reference value (see Challenge 1) for the impacts to define whether or not a chemical is SSbD. Therefore, a consistent way to deal with them is necessary. In the current work, it was possible to identify the following cases:

1)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 plasticisers case study, for which many applications are possible, but we defined the gasket manufacturing as the specific one assessed.

2)Another case is when a comparison is made between the same chemical obtained from different supply chains (e.g. different production processes, raw materials, or both). It is important to note that if a chemical is produced through different processes, this may lead to differences in properties that affect its use for the final application, such as concentration, impurities, or colour. Therefore, if it can be proven that there is technical equivalence between the chemicals (i.e. they can be perfectly substituted in all final applications), it is theoretically possible to establish a comparison at the intermediate level as well. A possible example is the assessment of the plasticisers derived from different feedstocks such as the

production of ATBC from bio-based butanol or the manufacturing of DEHT from recycled terephthalic acid. 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 fulfil 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)Another case is when one or more chemicals are used as reagents for another reaction. In this case, the functional unit is the ability to produce the desired final chemical (e.g. acetic acid and acetic anhydride can be used for the acetylation of another 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 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 modelling 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, since it shall encompass the whole life cycle. However, the information on the assessment at the intermediate level are crucial for the modelling of other chemicals or materials downstream of the analysed one. So, it is important that cradle-to-gate assessments are used and passed on 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, 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 which mix different chemicals to create the final product. In 2024, according to the European Chemical Agency (ECHA), more than 22000 substances are registered in REACH (ECHA, 2024).

Having an updated and technologically representative modelling 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 applying the SSbD framework and performing LCA of their portfolios.

To address this challenge, data gap estimation procedures have been proposed in literature. Parvatker & 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 is 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 target ones) and the Molecular Structure based Models (MSM) may be considered as viable options only for the modelling 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 & Eckelman (2019) hierarchy). If this assumption is verifiable, thus there is enough information on the chemical under assessment to conclude that 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 & Eckelman (2019)). On the other side, if the assumption cannot be verified then it may introduce strong biases in the model.

Regarding SMSs, 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 MSMs is also pointed out by Langhorst et al. (2023). In contrast, they quantitively 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 trade-off between accuracy and time resources used in modelling.

An intermediate strategy developed recently by Langhorst et al. (2025) consist in a machine learning algorithm that estimates life cycle inventory flows from the stoichiometric data of a chemical reaction. While this approach may seem similar to the MSMs it has two major points of improvement. It feeds the algorithm also with information on the precursors of the desired chemical and it estimates gate-to-gate inventories, which determines a stronger causal relation compared to MSMs.

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 feedstocks) or when the market condition changes in the Oil market. For example, the development of shale gas fields in the US, 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 member 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 products. 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 number of public LCA profiles for chemicals will also be beneficial to build extensive databases to train Machine Learning algorithms as the one proposed by Langhorst et al. (2025).

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. In this case, the fate of the chemical or material in the specific application considered can be hard 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; then 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 modelling. Since this type of analysis usually joins statistics and data from different sources, together with specific knowledge on the collection and treatment of waste, they derive a more detailed model of the mass flows of waste in a sector (Amadei et al., 2023a).

3)Then, each chemical may lead to different emissions to 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 modelled 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.

For example, in the case study, the emissions due to the incineration of the plasticisers, the PVC, and the additives were modelled under the assumption mentioned. However, modelling the emissions of the plasticisers themselves into the environment requires several assumptions on the migration dynamic of the plasticisers from the PVC matrix and to air or water. In the SSbD context, this

modelisation can be done following the assessment of consumers' and workers' exposure, which is part of the safety assessment and modelling of the framework.

Finally, the emitted chemical shall exist in the list of available elementary flows and have a characterisation factor in the LCIA method. Otherwise, the inclusion of this emission in the LCI does not affect the final results (See Challenge 7).

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 both 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, that can be relevant in other parts of the life cycle.

For example, in the plasticiser case study, some plasticisers 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 modelling 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. 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 it is done with uncertainty parameters or geographical location. A step in this direction is the development of a more complex data structure, namely an ontology for LCA data, that 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 pre-market approach able to drive sustainable innovation in the chemical industry (EC, 2021b). In particular, 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 & development activities of companies. LCA is an already established method among companies to evaluate existing processes and technologies but 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 goal of being applicable to innovative processes. Since different applications often lead to very different scenarios and assumptions, it makes 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:

1)Definition of a Goal & scope, that is consistent among different applications

2)Lack of data to compile an LCI that is representative of the process at industrial scale

3)Scenario definition for relevant technological changes in time

4)Consistency of the foreground scenario assumed with the background datasets available

5)Difficulties in modelling 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. A tentative for bio-based products has been done (Cucurachi et al., 2022). However, the reflection should be extended to the rest of the chemicals and materials industry, to serve the SSbD purpose. Other attempts to apply 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 modelling. Sacchi et al. (2022) developed a methodology to adapt existing LCA database to future scenarios. While this approach can be extremely useful, currently requires the practitioner additional programming skill which hinder the usability, especially outside of the academia.

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

2.2.3.Life Cycle Impact Assessment

Challenge 7: Impacts from substances of concern

One of the important goals of the CCS and hence of the SSbD framework is to reduce the use of substances of concern (SoC). SoCs are chemicals that exhibit hazardous properties, such as toxicity, persistence and bioaccumulation, requiring special regulatory attention.

The goal of their reduction includes in not limited to SoCs as a direct object of the assessment but also analysing 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)Characterisation 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 modelling of the end-of-life from the practitioner side, when this information is not available. Indeed, if no information on the presence of a plasticiser is present in the background data, then it will not be possible to model its release in the environment while modelling the end of life of the building.

3)The manufacturing of SoC, 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 plasticisers, 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 plasticised 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 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.

2 Comparability of chemicals

Part of this chapter is already published in Ardente et al. (2022) as an analysis on the comparability of intermediate products in LCA.

As shown in the previous chapter, a key concept for the application of SSbD is comparability. Comparability allows to evaluate environmental performances of different chemicals or materials on a common basis and make decisions on which one is a better alternative to fulfil a given function. In short, it allows to define benchmarks based on the actual state of the market, (see option 2 proposed in the Challenge 1 section). Moreover, the chemicals are often intermediate products and therefore it is important to understand how LCA can be meaningfully applied to these cases, as discussed in Challenge 2.

The aim of this section is to assess if and how comparability of intermediate products could be achieved in LCA, following the rules of the Environmental Footprint, and how it could be further developed.

2.1 Comparability in LCA

According to the PEF method, comparability in LCA can be achieved only if the same functional unit[1] can be fulfilled by different products, and therefore the system boundaries shall include the whole life cycle (i.e. cradle-to-grave assessment). This is stated clearly in chapter A.3.2:

"*Meaningful comparisons may only be made if products are fulfilling the same main function (as expressed through the functional unit). Therefore, the scope of a PEFCR for final products should be defined based on the function, with any deviations to be justified.*".

Similarly, ISO 14040 states *"Comparisons between systems shall be made on the basis of the same function(s), quantified by the same functional unit(s) in the form of their reference flows".*

For intermediate products however, since they can fulfil different functions, it is difficult or impossible to define a functional unit, however following a material approach is common to use a declared unit. Therefore, PEF currently do not allow for the creation of benchmarks at intermediate levels.

A possible workaround is to consider a set of properties of the intermediate chemicals or materials, that allows to identify its compliance for one (or more) applications.

[1] The functional unit in the PEF methodology is defined as the quantified performance of the product system, which serves as a reference unit for the study.

2.2 Analysis on three categories of intermediate products

This possibility was investigated in Ardente et al., (2022) with three categories of materials: Cement, steel and polymers. For each material, a review of the existing technical standards and a scan of the related industry was conducted to understand how these materials are commonly classified at intermediate level and which information are used to communicate relevant information properties from the manufacturer to the customer. Then, a search through the most common sources of LCA studies of commercial product was conducted to look for evidence that such approach is meaningful for the industry.

For cement, it was found that a European technical standard (EN-197-1) describes the classification of cements based on chemical composition) and compressive strength. This type of classification is deemed relevant, since it is reflected in the additional information reported in publicly available Environmental Product Declaration. Finally, the evidence collected from technical standards and industry allow us to propose a classification for comparability purposes that is based on the mentioned criteria. This classification is based on the connection between relevant technical properties (i.e. the compressive strength and composition) with the potential functionality of cement in the final application. Figure 5 shows the classification of cement in EN 197-1.

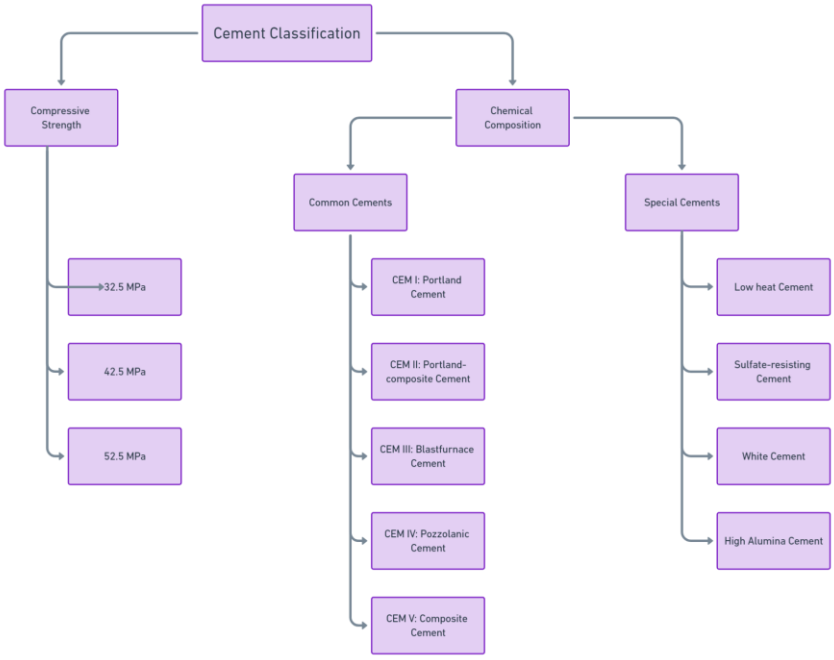

Figure 6. Simplified classification of cements based on chemical composition from EN 197-1.

A similar approach has been applied to the steel sector and the polymers. Similarly to the cement, In EN 10027-1, Category 1 steel nomenclature is a systematic approach that provides information about the steel's properties based on its intended application. The nomenclature consists in the first letter, which indicates the general application, a two-digit number, which indicates the value of

a relevant mechanical property (usually yield strength) and an additional alphanumeric symbol, which gives information on another technical property or type of heat treatment.

For example, the nomenclature S355J2 would refer to a structural steel with a yield strength of 355 MPa and impact strength tested at -20°C. In Table 19 the eleven application classes, with their letter and relevant property are shown.

Table 19. Summary of the application classes defined in EN 10027-1

Application	Letter	Relevant mechanical property
Structural steel	S	Minimum Yield Strength
Pressure purposes	P	Minimum Yield Strength
Line pipe	L	Minimum Yield Strength
Engineering Steel	E	Minimum Yield Strength
Steel for reinforcing concrete	B	Characteristic yield strength
Steels for prestressing concrete	Y	Nominal tensile strength
Steel for or in the form of rails	R	Specified minimum Brinell Hardness
Flat products for cold forming	D	Symbol for Hot/cold rolling
Flat products of high strength for cold forming	H	-
Tin mill products (steel products for packaging)	T	nominal yield strength
Electrical steel	M	max specified loss

In the second designation system, which is based on chemical composition, there are four groups of steel, each following distinct naming conventions. These groups are represented by a symbol, including a number indicating the percentage of carbon in the steel, followed by a string of chemical symbols representing the alloying elements and their concentrations. Table 20 outlines the naming rules for all four steel groups, along with an example taken from the standard.

Table 20. Nomenclature system category 2 based on chemical composition

Steel alloy	Main symbol	Example
Non-alloy steels (except free cutting steels) with an average manganese content < 1 %	Percentage of Carbon multiplied by 100	C35
Non-alloy steels with an average manganese content ≥ 1 % or alloy steel with <5% of one alloying element	Percentage of Carbon multiplied by 100 + chemical symbols of alloying elements followed by their percentage multiplied by a conventional factor (4 for Cr, Co, Mn, Ni, Si, W 10 for Al, Be,Cu, Mo, Nb,Pb, Ta, Ti, V, Zr; 100 for Ce, N, P, S; 1000 for B)	13MnNi6–3
Stainless steel with more the >5% of one alloying element	X symbol + percentage of Carbon multiplied by 100 + chemical symbols of alloying elements followed by their percentage	X38CrMoNb16
High speed steel	HS symbol followed by numbers indicating, in the order, the percentage content of Tungsten, Molybdenum, Vanadium and Cobalt	HS2–9-1–8

This classification system does not consider mechanical properties of steel, and therefore is difficult to link a steel nomenclature to its potential applications, unless the chemical composition leads to specific properties (e.g. corrosion resistance) required in niche applications. Hence, its applicability for comparative purposes is less relevant than the first classification, but could be used to complement it.

The first classification system, instead, could allow to link different types of intermediate steel products with possible applications.

Investigating the steel industry for LCA applications, showed mixed results. The international association Worldsteel develops LCA profiles for intermediate steel products (Worldsteel, 2024) in which the products are differentiated based on processes and shapes (e.g. cold rolled coils or rebars) with a weak connection with the final intended use. Similarly, existing Environmental Product Declarations (EPD) follow the same type of categorisation.

Regarding polymers, they exhibit a wide range of properties and are typically traded in granulate form. After production, polymers may be mixed with additives or other polymers to optimize them for specific uses, posing challenges for comparability. This complexity is further amplified by the growing importance of bio-based polymers, which can either be entirely new or traditional polymers made from bio-based feedstock. These differences in supply chains necessitate unique rules for LCA to allow meaningful comparisons between fossil-based and bio-based polymers.

Comparability between polymers could be based on technical properties such as tensile strength, glass transition temperature, melting temperature, and melt flow rate, which influence both the final use and the manufacturing phase. For widely used polymers like PE, PP, PET, and PVC, melt flow rate is a critical property that affects manufacturing processes and final applications. Classifying polymers by type and melt flow rate to reflects technical needs for different manufacturing processes could serve as a basis for comparability. However, in the industry, LCA is often applied by considering only the type of polymer (e.g. PE, PP etc.) as it is done in the PlasticsEurope eco-profiles, or by adding few information on mechanical and technological information as it is done in EPDs (IES. 2026).

2.3 Discussion

Finally, this chapter explored the challenges of ensuring comparability of intermediate products within LCA and Environment Footprint, emphasizing that meaningful comparisons depend on the ability to establish a strong relationship between the intermediate product’s properties and its final use. It is generally difficult to derive universally valid conclusions for all intermediate products due to the diversity of product categories and underlying technological processes. Thus, comparability needs to be addressed on a product-specific basis, requiring detailed market and technological knowledge.

For certain sectors, such as cement, comparability is more feasible. The European standard EN 197-1 offers an interesting solution by defining relevant properties that could enable the creation of a declared unit for comparing cement products. This standard is widely used for environmental declarations in the cement industry, indicating its usefulness in describing key material properties to the end-user.

In contrast, the comparability of steel products could be defined using the EN 10027-1 standard, which categorizes products into 11 groups and defines performance based on mechanical properties. However, other LCA initiatives in the steel industry often use higher levels of aggregation for environmental communication, which raises questions about the practicality of this approach for industry-wide adoption.

For polymers, defining comparability remains challenging due to difficulties in establishing technical specifications that meaningfully reflect intended uses. A potential solution is to compare polymer products that share the same key technological properties, though further investigation is needed to link these properties to final use.

The document also highlights that as the number of parameters used in defining comparability increases (e.g., mechanical properties, composition), the link between intermediate products and their final use becomes stronger, but managing these parameters becomes more complex. This complexity could result in a high granularity level, which could make the comparison less meaningful.

The PEF method currently prohibits benchmarks for intermediate products, but the analysis suggests that this could be reconsidered, at least in the SSbD context, if relevant comparability criteria for specific product categories are identified. Although, when possible, a complete cradle-to-gate LCA should be preferred.

3 LCA Data in the chemical industry: a tool for rapid proxy building

The supply chains of the chemical industry are inherently complex due to several interrelated factors. First, the production of chemicals often involves multiple stages, with raw materials undergoing various transformations and refinement processes before resulting in the final product. These processes frequently span different geographical regions, involve numerous suppliers, and require a diverse array of intermediates and energy inputs. Additionally, the globalized nature of the chemical industry, with extensive networks of subcontractors, makes traceability of material flows difficult. Another source of complexity is the significant variety of chemicals and their associated production methods, as different chemicals require distinct synthesis routes, feedstock, and technologies.

The application of Life Cycle Assessment (LCA) to the chemical industry faces substantial challenges due to the aforementioned supply-chain complexity. LCA aims to quantify the environmental impacts of a product or process across its entire life cycle, from raw material extraction to disposal. In the case of chemicals, accurately modelling the entire supply chain is challenging due to the multistage processes, numerous intermediaries, and global scale of production. Each stage requires precise data on energy consumption, emissions, resource use, and waste generation. Additionally, the extensive use of intermediate chemicals in various industries, such as pharmaceuticals, agriculture, and plastics, means that interlinkages between different supply chains must also be accounted for, further complicating the assessment.

Despite this, many chemicals are fossil-based, hence they share a common origin in their supply-chain since they all come from oil, gas or coal. In particular, these natural resources are often used to obtain a limited number of different basic chemicals, which are produced worldwide in huge quantities and then are used to manufacture more complex chemicals or materials, such as plasticisers or plastics.

Moreover, basic chemical processes based on fossil feedstock are quite mature since they were developed years ago and did not change significantly in recent time. Therefore, even if details on process operational conditions, catalyst and separation techniques may change, the overall mass balance can be drafted for many of this process based on available scientific literature.

In the following section it will be shown how to leverage this feature of the industry to develop an Excel-based tool to explore and visualize supply chains of chemicals. This tool can provide assistance in modelling LCA proxy data, or to

quickly understand on which natural resources a chemical relies, and therefore potential savings in substituting it with an innovative chemical or with a different process to manufacture it.

In the next section, a brief explanation on the mathematical theory behind LCA is provided. In section 3.2, then is illustrated how the tool is built based on that theory.

3.1 LCA Mathematical structure

Life cycle assessment, from the mathematical point of view, is based on linear algebra. The basic building block is the representation of a unit process[2]. A process is an activity that generates one (or more) output from multiple inputs. These inputs and outputs can be represented with a one-dimensional vector of numbers. For example, let's consider the process of burning natural gas to produce electricity. The position in the vector identifies the type of input/output flow, while the number indicates its amount and its sign the direction of the flow (positive for output, negative for input). Following the notation from (Heijungs & Suh, 2002):

$$\boldsymbol{p_1} = \begin{pmatrix} kg\ of\ natural\ gas \\ kg\ of\ \ CO_2 \\ kWh\ electricity \end{pmatrix} \begin{pmatrix} -0.25 \\ 0.7 \\ 1 \end{pmatrix} \qquad 1$$

In Equation 1, the vector tells us that to produce 1 kWh of electricity, 0.25 kg of natural gas is needed and 0.7 kg of CO_2 are produced as an output. This approach reduces a process to a point in an n-th dimensional linear space. Where n is the number of flows considered.

If we need to know how many kg of CO_2 are emitted to produce 15 kWh we multiply the vector for a scalar (15) that represent a scaling factor for the vector $\mathbf{p_1}$.

However, if we want to go further and understand which natural resources are used and which kind of emissions are generated across the supply chain of the electricity, it is necessary to expand our analysis to include also the process of natural gas extraction. And so forth until we have considered all the processes involved in the supply chain of the electricity generation.

To do so, we expand the list of our processes to a larger set of processes, and our vector basis accordingly, to include all the elementary flow needed. Following this procedure, we get a larger matrix that has all the unit processes on the columns and a row for each existing flow needed for the set of processes considered. Let us consider the vector in Equation 2 for the production process of natural gas $\mathbf{p_2}$:

[2] In ISO 14040 unit process is defined as the smallest element considered in the life cycle inventory analysis for which input and output data are quantified.

$$\boldsymbol{p_2} = \begin{pmatrix} kg\ natural\ gas \\ kWh\ electricity \\ kg\ of\ raw\ natural\ gas \\ kg\ of\ CH_4 \end{pmatrix} \begin{pmatrix} 1 \\ -0.1 \\ -1.1 \\ 0.1 \end{pmatrix} \quad 2$$

And let's create the matrix P by juxtaposition of p_1 and p_2, and by adding zeros for the missing flows in two vectors.

$$\boldsymbol{P} = (\boldsymbol{p_1}|\boldsymbol{p_2}) = \begin{pmatrix} kg\ natural\ gas \\ kWh\ electricity \\ kg\ of\ CO_2 \\ kg\ of\ CH_4 \\ kg\ of\ raw\ natural\ gas \end{pmatrix} \left(\begin{array}{c|c} -0.25 & 1 \\ 1 & -0.1 \\ 0.7 & 0 \\ 0 & 0.1 \\ 0 & -1.1 \end{array}\right) \quad 3$$

Among the existing flows visible in Equation 3, we can differentiate two groups: one is the group of flows that represents products or services that are exchanged between economic activities inside the human economy; the second is the group of flows representing an exchange between the environment and the economic system (e.g. emission of substances to air, extraction of natural resources). These are often named technical flows or intermediate flows and elementary flows respectively.

Sorting the rows to separate the technical flows from the elementary flows it is possible to obtain two submatrices **A** and **B**. **A** is named technology matrix since it contains all the flows exchanged within the economic system. It is important to say that each process in **A** must be associated to a single product flow. This requirement is needed for **A** to be a square matrix.

B is named intervention matrix since it represents the environmental intervention of each unit process, i.e. the exchange happening directly with nature (e.g. emissions in atmosphere or water withdrawal). None or many of this exchange may be associated to one process, hence **B** is a rectangular matrix with the same number of columns as **A**.

$$\boldsymbol{P} = \left(\frac{\boldsymbol{A}}{\boldsymbol{B}}\right) = \begin{pmatrix} kWh\ electricity \\ kg\ natural\ gas \\ \hline kg\ raw\ natural\ gas \\ kg\ CO_2 \\ kg\ CH_4 \end{pmatrix} \left(\begin{array}{cc} 1 & -0.1 \\ -0.25 & 1 \\ \hline 0 & -1.1 \\ 0.7 & 0 \\ 0 & 0.1 \end{array}\right) \quad 4$$

With the matrix sorted as in Equation 4, we can approach the inventory problem and answer the question of *how many exchanges with nature are needed to obtain a defined quantity of a product*. In the example above, let us see how much natural gas is needed and how much carbon dioxide is emitted to produce 1 kWh of electricity. To do so, let us define the demand vector **f** as vector as long as

the number of processes included in the technology matrix **A** (2 in our example), and with the number f_i .

$$\boldsymbol{f} = \begin{pmatrix} f_i \\ \dots \\ 0 \end{pmatrix} with\ f_i = desired\ amount\ of\ i^{th}\ intermediate\ flow \quad (5)$$

Now, we want to know how much each process needs to be scaled up by a number, to meet the demand **f**. which translate into the multiplication of matrix **A** by a scaling vector **s**:

$$\boldsymbol{As} = \boldsymbol{f} \Rightarrow \boldsymbol{s} = \boldsymbol{A}^{-1}\boldsymbol{f} \quad (6)$$

Solving this linear system shown in Equation 6, we get the amount of each process in A needed to obtain the desired quantity of f. In our example, for a f=1 kWh of electricity

$$\boldsymbol{s} = \begin{pmatrix} 1.026 & 0.103 \\ 0.256 & 1.026 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1.026 \\ 0.256 \end{pmatrix} \quad (7)$$

Meaning that the 0.256 kg of natural gas needs to be used to generate 1.026 kWh of electricity used to meet the final demand of electricity and the production of natural gas itself. Finally, to obtain the list and quantity of elementary flows underlying the intermediate flows we can use the intervention matrix B following the equation 8:

$$\boldsymbol{g} = \boldsymbol{Bs} = \begin{pmatrix} 0.28 \\ 0.72 \\ 0.026 \end{pmatrix}\begin{pmatrix} kg\ raw\ natural\ gas \\ kg\ CO_2 \\ kg\ CH_4 \end{pmatrix} \quad (8)$$

Hence, to generate 1 kWh of electricity from natural gas, the whole supply-chain of processes will extract 0.28 kg of natural gas and release 0.72 kg of CO_2 and 26 g of CH_4.

Therefore, to summarise, the equations that solve the inventory problem are:

$$\begin{cases} \boldsymbol{s} = \boldsymbol{A}^{-1}\boldsymbol{f} \\ \boldsymbol{g} = \boldsymbol{sB} = \boldsymbol{A}^{-1}\boldsymbol{Bf} \end{cases} \quad (9)$$

While s is obtained solving a linear system, it only represents the set of all the technological flows needed to fulfil the demand of product defined by f. Instead, g represents the whole set of exchanges between human activities and nature along the life cycle of the product requested. This constitute the base of LCA since the vector **g** is then used to calculate environmental impacts, such as Climate Change, in the LCIA phase with the multiplication of each element of the vector (representing an emission or an input) by a number called Characterisation Factor which quantifies the effect of that flow on the associated environmental impact using a common unit of measure (e.g. kg CO_2eq.).

3.2 Methodology

Given a technology matrix $\boldsymbol{A}$, rows and columns can be rearranged to separate processes that use as a raw material a fossil natural resource to produce a chemical and processes that produce chemicals from other ones. This allows to identify a set of chemical building blocks that are at the beginning of the supply-chains included in the technology matrix $\boldsymbol{A}$. Figure 7. shows how the technology matrix A is split into 4 sub-matrices:

1. A petrochemical technology matrix, which contains all the process going from oil, gas or coal to individual chemicals. These chemicals will be called building blocks. The matrix is n×n square matrix (n processes for n building blocks).
2. The chemical industry matrix, from now named $\boldsymbol{C}$, is a square matrix which contains all the process to produce chemicals, except for the building blocks.
3. A rectangular matrix, from now named $\boldsymbol{D}$, which contains all the flows of building blocks used in the chemical processes. The matrix has m columns, like the chemical industry one, and n rows as the number of building blocks.
4. The remaining rectangular matrix comprises any use of chemicals in petrochemical processes and it is not of interest for the goal of this work.

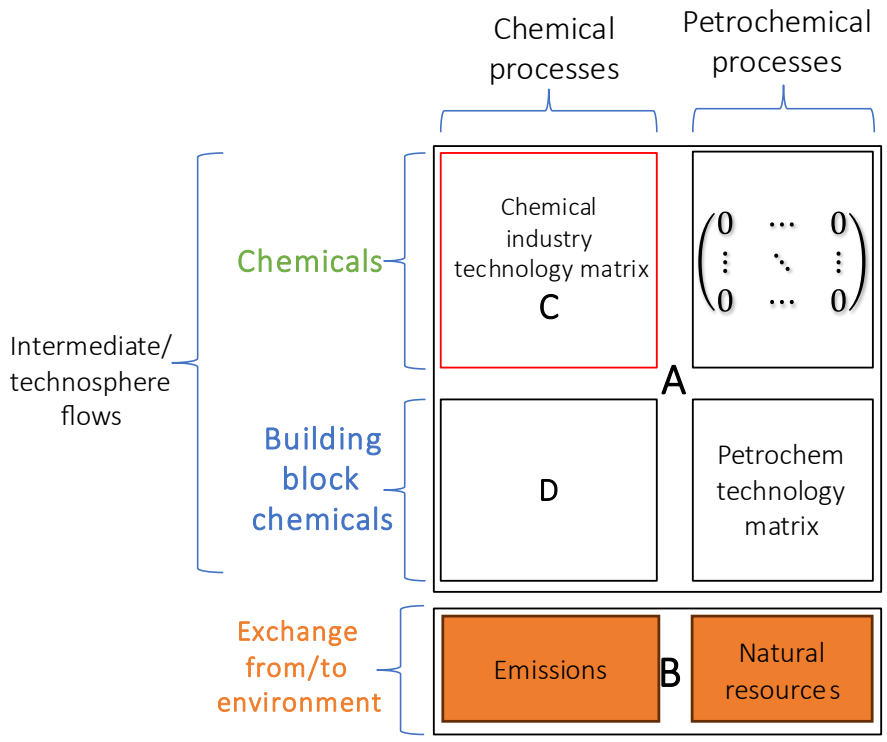

Figure 7. Visualisation of the technology (A) and intervention matrix (B) and their submatrices

It can be noted that the chemical industry matrices described in point 2 and point 3 represent a smaller version of the life cycle inventory problem described in section 3.1. By solving the linear system:

$$\begin{cases} \boldsymbol{s' = C^{-1} f} \\ \boldsymbol{g' = s' D} \end{cases} \quad 10$$

We get the amount of building blocks needed to produce a desired amount of a chemical. With this decomposition is possible to generate an "industrial footprint" of the supply-chain of a chemical showing the composition of the chemicals as sum of building blocks.

3.2.1 Chemical industry technology matrix creation

In order to identify a limited subset of relevant chemicals to be mapped into the tool, it was decided to consider production volume as a first screening criterion. To do so, the most relevant data source identified was ECHA.

REACH Regulation is the main European regulation on chemicals, it requires mandatory registration of chemical substances from producers or importers in order to identify the risks coming from the presence of a chemical on the market. The list of all the registered chemicals was retrieved from the ECHA website (ECHA, 2025) to select a starting group of chemicals to build up the base of the tool. Currently, the list accounts for more than 26000 items.

The first criteria to select a subset of substances is the tonnage band, i.e. an estimate of the whole production at European level in mass. Tonnage bands over the 100.000 ton were selected. Additionally, all the registered substances which cannot be identified directly with a molecule (e.g. gasoline), inorganic substances such as mineral and metals were excluded from the scope of the analysis. Exceptions to these criteria are made to include chemicals that are needed to complete the supply-chain of another one (e.g. Hydrochloric acid). Moreover, basic polymers were added to the set despite not being included in the REACH registration database.

Chemicals identified with these criteria were mapped with their CAS identifiers and basic properties such as the Molecular weight. Then, for each of them a production process was identified in literature. The main sources of industrial chemistry literature were the Ullman's and the Kirk-Othmer Encyclopaedias (*Kirk-Othmer Encyclopedia of Chemical Technology*, 2000; *Ullmann's Encyclopedia of Industrial Chemistry*, 2003). Each industrial process was identified with a unique identifier and then a stoichiometric mass balance between reagents and products was set. For the purpose of the calculations, each process has a chemical defined as "Main output" and all the masses of chemicals involved are divided by the mass of the main output to be normalised. In Table 21 is shown an excerpt of the processes database to illustrate the data structure created.

Table 21. Example of the data structure of the chemical processes database

Process ID	Process	Main output	Input/output	CAS	Mass	Mass scaled	Mole
001	Amoco oxidation 1	Terephthalic acid	Terephthalic acid	100-21-0	166.13	1	1
001	Amoco oxidation 1	Terephthalic acid	Water	7732-18-5	36.0306	0.22	2
001	Amoco oxidation 1	Terephthalic acid	p-xylene	106-42-3	-106.168	-0.64	-1
001	Amoco oxidation 1	Terephthalic acid	Oxygen	7782-44-7	-95.997	-0.58	-3

After the mapping of 132 different substances and their production processes, 32 chemicals were identified as building blocks, since their production was the result of a direct extraction from a fossil resource (e.g. ethylene, benzene etc.) or basic elements coming from other natural resources (e.g. oxygen and nitrogen from air or Chlorine from sea salt), was possible to compile the matrix C and calculate its inverse.

With this operation is possible to solve the linear system and calculate the "industrial fingerprint" of the chemicals. In the following section, an example of use for the tool is presented.

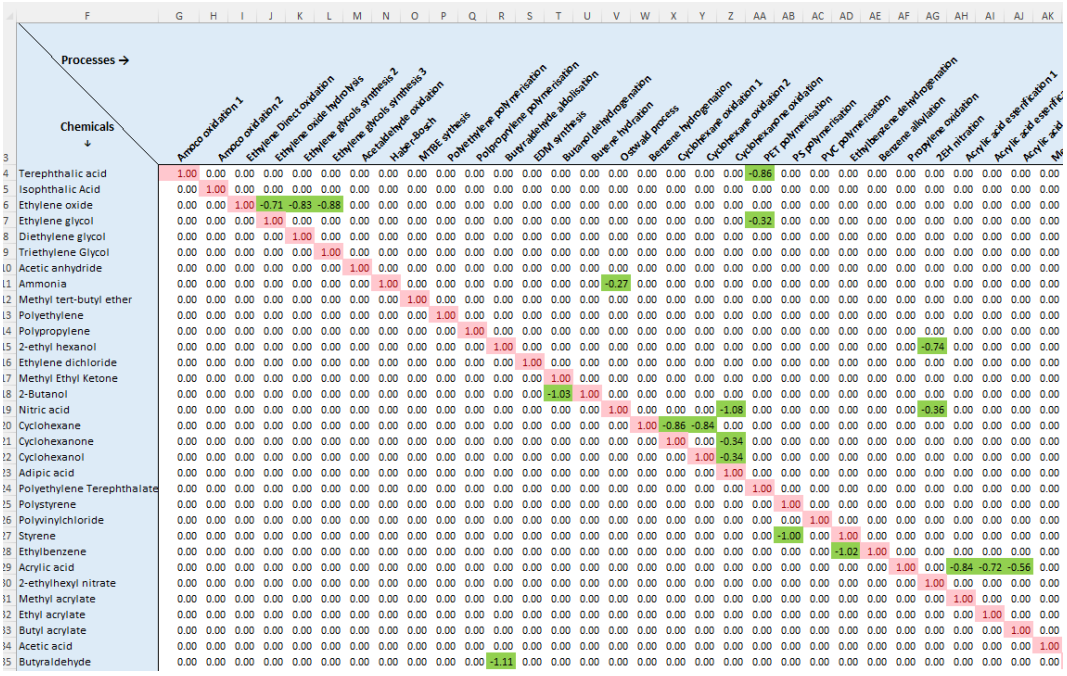

Figure 8. Excerpt of the C matrix developed

3.3 Application to the plasticiser case study

To test the tool, it was decided to calculate the industrial fingerprint of five of the six plasticisers of the case study presented in Chapter 1. The ESBO, was left out of the analysis, since it is almost entirely made from biomass. Also in this case, to properly compare the chemicals, the same criteria used in Chapter 1 are used. In particular, 1 kg of DEHP is considered as the reference quantity, while for the other plasticiser this quantity is multiplied by the substitution factor from Table 1.

It can be seen that the similarities in the structure of the plasticiser are reflected in their supply-chain, especially for the DEHP and DEHT, which have the exact same supply-chain, starting from two different isomers of the xylene. The total amount of building blocks needed differs because of the higher amount of DEHT needed to replace 1 kg of DEHP. The ATBC shows a lower amount of chemical building blocks compared to the others, due to its citric acid content, which is made from biomass and therefore is out of the scope of the tool.

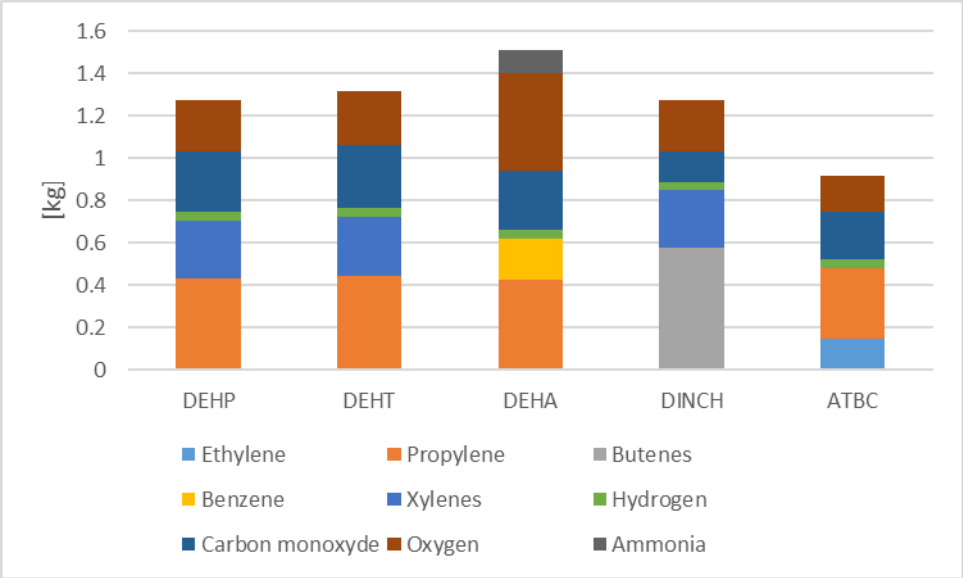

Figure 9. Mass of chemical building blocks for 1 kg of Di ethylhexyl phthalate and the equivalent amount of its potential alternatives.

3.4 Discussion

The methodological approach behind this tool provides a quick way to understand and explore the supply-chain behind a chemical, showing potential benefits from substitution between chemicals or between different processes to obtain the same chemical (e.g. through the inclusion of bio-based version of one or more precursors). Moreover, since the information required to conduct such analysis is limited, it can provide valuable insights even at early-stage in the R&D process and before a proper LCA is set for the SSbD application.

For example, in the case of plasticiser, the analysis shows a small difference between DEHP and DEHT which may suggest that a limited benefit can be achieved from the substitution of the phthalate plasticiser with the terephthalates. However, in the supply-chain of DEHT the terephthalic acid is involved, which can be potentially sourced from chemical recycling of PET. In that case, a significant part of the "industrial footprint" of the DEHT would disappear and potentially lead to lower LCA impacts.

At the present stage of development, only the stoichiometric amount of reactants and products is considered without accounting for process losses due to purification steps, impurities, side-reactions and other non-ideal conditions occurring in a real plants. Moreover, the amount of fossil resources used to

provide energy to the processes is excluded, since it may change significantly in different plants due to different level of energy integration in the facility and its localisation. This aspect is better addressed in a full LCA analysis and therefore left out of the scope of the tool.

A good overview of the global chemical supply-chain is presented by Levi & Cullen (2018), where they performed a Mass Flow Analysis of the most relevant commodity chemicals globally. While it is a very instructive study, it does not easily link with the need of an SSbD practitioner which may need to investigate the specific supply-chain of a fine chemical.

This tool can be seen as complementary to some of approaches mentioned in Challenge 4, for data gap filling. For example, while Parvatker & Eckelman (2019) provide a hierarchical approach on how to model processes with insufficient data, the present approach provides a map of the chemical supply-chains to guide its application. Similarly, it could be used with the tool developed by Langhorst et al. (2025) to retrieve all the synthesis step in the supply-chain of a chemical and estimates simple inventories for each of them. In case of the choice the use of an existing process as proxy for another, the tool can allow the comparison of the two supply-chains instead on relying on debatable assumptions such as for the molecular structure.

4 Dataset adaptation to future scenarios

In the present chapter will be presented the author contribution to a study focused on plastics. The author contributed with the conceptualisation and adaptation of the LCA datasets of plastics to better represent technological and geographical differences.

In the study, a Mass Flow Analysis based on Amadei et al. (2023b) was used as a base for developing a sector wide LCA. This LCA estimates the environmental impacts of European plastic consumption, considering nine different plastics. In this analysis it was necessary to: 1) improve the representativity of plastic production out of EU (to model the import) and 2) model the possible changes in environmental impacts of future plastic production due to the change in the energy mix. To do so, different sources of data were used to adapt existing Ecoinvent datasets to the required scenarios.

This kind of modelling is relevant in the SSbD scenario, since innovative processes or supply-chains may not have the sufficient amount of data to be modelled in LCA or may require to be realistically evaluated at a future point in time in which the technology is industrially available (See Challenge 6).

4.1 Methodology

The first goal of the analysis was to understand the amount and the source of European plastics import. This exercise was applied to the four most relevant plastics included in the paper. Namely, Polyethylene (high and low density), polypropylene and polyethylene terephthalate.

For the first goal, we started estimating the impacts arising from the import of virgin polymers, the quantities and countries of origin of imported polymers in the EU was needed. In the first place, this information was retrieved from the World Integrated Trade Solutions database (World Integrated Trade Solutions, 2024) using a 6-digits Harmonized System (HS) Code (an internationally standardised numerical classification system used for products importing) for each polymer.

From this source, it was possible to quantify the total amount of polymers imported in European Union in 2019 as 6.87 Mt, (13% of the total 53 Mt produced estimated in Amadei et al. (2023a). Of this, the selected four polymers represent 85% of the total import.

Then, for each of the four polymers the top five source countries were considered as representative of the whole import. Table 22, shows the countries of

origin for each polymer. Starting from this list, two modifications to the original polymer dataset were done:

1. Transport mode and distances: Instead of using an average transport scenario from outside EU, the transport via transoceanic ship was calculated assuming a main port in the country of origin, and calculating the shortest one between Rotterdam and Genova. The distances were calculated through the website Sea-distance.org (Sea-distance.org, 2026). These two European cities were chosen to represent the two main sea-courses for goods reaching Europe through the Atlantic Sea (Rotterdam) or the Mediterranean Sea (Genova). Transport on road was modelled using a truck (>32t) for an assumed distance of 1000 km as in Nessi et al. (2021 a, b)).
2. Plastic production impacts: to improve the geographical representativeness of the four imported polymers the EU ecoinvent dataset for the production of each polymer was adapted considering the five countries of origin. To do so, the quantity of electricity and heat in input was allocated to the five countries of origin proportionally to share o import (see Table 23) and associated to the available country-specific dataset for electricity and heat. Where the specific geography was not available in the database, the 'Rest of the World' dataset was used.

Table 22. Top five countries of origin for the imported polymers and their share of the total import

HDPE		**LDPE**		**PET**		**PP**	
Country	**Share**	**Country**	**Share**	**Country**	**Share**	**Country**	**Share**
Saudi Arabia	35%	Saudi Arabia	29%	South Korea	28%	Saudi Arabia	53%
United States	32%	United States	24%	China	24%	South Korea	23%
Egypt	13%	Qatar	20%	India	20%	South Africa	8%
Brazil	12%	South Korea	16%	Turkey	18%	Egypt	8%
Qatar	8%	Norway	11%	Indonesia	11%	India	7%

In the second goal, a scenario was developed to explore the expected change in electricity and heat mixes at European level. Two different energy mixes were modelled to represent a policy target scenario and a more ambitious one:

1. The future electricity mix (*Mix 1)* was calculated analysing the expected trends in electricity generation described in Keramidas et al. (2021), EC (2019a) and Garcia Gutierrez et al. (2023), based on policy targets (such as those in the 'European Green Deal' (EC, 2019)).
2. The electricity *Mix 2* instead was calculated considering a more ambitious target in terms of share of renewables compared to *Mix 1*.

The current energy mix for the electricity were derived from the analysis of the process contribution to the Ecoinvent dataset "*Electricity, medium voltage {RER}| market group for | Cut-off, U*", which is the dataset used along the whole

study. A summary of the composition of the two scenario mixes and the base is provided in Table 23.

The heat mix for the current scenario was derived from Garcia-Gutierrez et al. (2023b). The heat mix shares for *Mix 1* and *Mix 2* are calculated from the same references of the electricity ones. Table 24 presents a summary of the and heat mixes composition.

Finally, the modified mixes were substituted to the base one in the life cycle, to show the effects on the final impacts.

Table 23. Electricity mix used in the base scenario and sensitivity mixes Mix 1 and Mix 2

Technology [share]	Electricity Base	Sensitivity 'Mix 1'	Sensitivity 'Mix 2'
Nuclear	29.80%	25.30%	19.40%
Natural gas	13.90%	12.80%	4.50%
Oil	1.60%	1.20%	0.40%
Lignite	11.10%	4.40%	0.00%
Hard coal	13.30%	5.20%	0.00%
Wind	10.70%	16.20%	24.60%
Hydro	15.40%	16.60%	22.90%
Solar	0.20%	11.80%	19.30%
Biomass	3.60%	6.00%	8.30%
Geo-thermal	0.20%	0.40%	0.60%
Note		Based on Keramidas et al. (2021),Garcia Gutierrez et al. (2023)	Based on Keramidas et al. (2021),Garcia Gutierrez et al. (2023)

Table 24. Details on the thermal energy mix considered for the base scenario and sensitivity mixes selected Mix 1 and Mix 2

Technology [share]	Thermal energy 'Base'	Sensitivity 'Mix 1'	Sensitivity 'Mix 2'
Natural gas	43.4%	37.2%	17.1%
Hard coal	27.3%	10.7%	7.7%
Biomass	25.8%	32.8%	62.2%
Heavy fuel oil	3.5%	2.9%	1.9%
Note	Based on Garcia-Gutierrez et al. (2023).	Based on Keramidas et al. (2021),Garcia Gutierrez et al. (2023).	Based on Keramidas et al. (2021),Garcia Gutierrez et al. (2023).

To show the potential effects of a shift to a different electricity and heat mix, the Mix 1 and Mix 2 shares were employed in the calculation of the whole value chain impacts, hence including the plastic production and manufacturing and the electricity substituted from the energy recovery happening in incineration facilities.

It is important to mention that the present scenarios assumed that the shifts in energy mixes happens only within EU, therefore excluding the potential effects of

changes of changing energy generation in the extra-EU part of the supply-chains. This is a conservative assumption leading to an underestimation of environmental benefits, since it is likely that also the rest of the world will reduce the environmental impacts of their energy mixes.

A relevant methodological aspect is to substitute the current energy mix from the background dataset, without double-counting in the whole supply-chain (i.e. not only the final energy needed to manufacture plastic products but also all the nested contribution in the upstream. For this reason, the author developed a procedure to calculate the exact quantity of European electricity, to be substituted.

For the replacement of the electricity mix the following approach was applied:

1. For each polymer, the process contribution of its production dataset was extracted from the Simapro software (e.g.: "Polyethylene terephthalate, granulate, amorphous {RER}| production | Cut-off, U"; "Polyethylene, low density, granulate {RER}| production | Cut-off, U"; etc.).
2. Analysing the Ecoinvent datasets, a set of high voltage electricity genearion was identified, including all countries included in the RER geography. These datasets were characterized in SimaPro using EF3.1 method and the. Choosing the high voltage datasets is important to avoid double-counting of electricity due to the complexity of the Ecoinvent modelisation of electricity generation, transmission and consumption.
3. For each process at point 1, the specific amount of electricity coming from each process identified in point 2 was noted. For instance, in the case of the "*Polyethylene terephthalate, granulate, amorphous {RER}| production | Cut-off, U*" dataset, the process contribution of the underpinning dataset "Electricity, high voltage {AL}| market for electricity, high voltage | Cut-off, U" amounts to 0.00248 MJ/kg_{PET}.
4. Multiplying the energy intensity (in MJ/kg) requirement for each polymer production process (point 1) and each relevant electricity production dataset (point 2), it was possible to calculate the impacts due to each specific electricity generation dataset in the current model of each polymer.
5. The sum of all the contribution calculated as in point 4 for all the datasets selected in point 2 was calculated. For instance, in the case of the "*Polyethylene terephthalate, granulate, amorphous {RER}| production | Cut-off, U*" dataset, the total contribution for the Climate Change impact category amounted to 0.173 $kgCO_2eq./kg_{PET}$ impacts due to the sole electricity needs of the process.
6. The impacts calculated in point 5 were then subtracted to the total impacts of the MFA, to be substituted with the impacts ariging from the use of Mix1 or Mix2 for the total amount of electricity calculated in point 4.

For the replacement of the heat mix during the production stage, the same approach described for the polymers' production was used. However, the list of dataset considered in point 2 were replaced with the following: "*Heat, district or industrial, natural gas {RER}| market group for | Cut-off, U*"; "*Heat, district or industrial, other than natural gas {RER}| market group for | Cut-off, U*", "*Heat,*

from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | Cut-off, U".

The same methodology was used to replace the heat and electricity mixes during the manufacturing stage, considering the datasets related to the injection moulding and extrusion instead of the polymer-specific production processes.

4.2 Discussion

This chapter presents a methodological contribution to the enhancement of Life Cycle Assessment (LCA) models used to evaluate the environmental impacts of plastics at the European scale. By addressing the representativeness of plastic production outside the EU and by exploring the influence of future energy scenarios, the work tackles two critical aspects of LCA modelling for policy-relevant applications: geographical specificity and prospective assessment.

Trade data represents a significant source of information toward improving the spatial accuracy of import-related emissions.

In particular, associating the four major polymers—HDPE, LDPE, PET, and PP—with country-specific electricity and heat mixes enables a more nuanced representation of the upstream supply chains. This level of granularity is particularly relevant when assessing systems with high shares of imports, or with very similar production processes, in which main differences may arise from the geographical context. The adapted datasets allow for the identification of environmental hotspots not only within European production systems but also in non-EU supply chains, which are often overlooked in standard LCA models due to data limitations.

Additionally, the development and implementation of future energy scenarios, through two distinct electricity and heat mixes (Mix 1 and Mix 2), allows for a forward-looking perspective in LCA modelling. This is particularly aligned with the goals of SSbD, which requires the evaluation of emerging technologies or supply chains under future, more sustainable contexts. By replacing current energy datasets with scenario-specific alternatives, the analysis captures potential environmental benefits that could arise from the decarbonisation of European energy systems. The applied methodology ensures that electricity and heat contributions are correctly associated, avoiding inconsistencies or double-counting, at the best of the possibility given by the disaggregated structure of the Ecoinvent database.

The findings also emphasize the importance of modelling flexibility in LCA tools. As supply chains evolve, both in terms of geographic distribution and technological configuration, LCA models must be adaptable. The methodology developed here supports such adaptability by demonstrating how existing inventory data can be modified using transparent and reproducible rules. This is particularly relevant in the SSbD context, where many innovative processes are not yet commercialized, and proxy-based or scenario-driven modelling becomes essential.

However, it is important to acknowledge some limitations of the approach. The analysis focuses on changes in energy mixes only within the EU, assuming static conditions in non-EU countries. While this is a conservative and methodologically cautious assumption, it may underestimate the environmental benefits associated with global decarbonisation trends. Furthermore, the approach relies on existing Ecoinvent datasets, which may not fully reflect process-specific technological variations in different countries or regions. Despite these

constraints, the approach provides a robust and scalable framework that could be extended in future studies to include dynamic non-EU scenarios or technological variants.

In summary, the work presented in this chapter contributes to improving the geographic and temporal relevance of plastic LCA modelling, offering a replicable methodology for LCA practitioners to enhance the representativeness and foresight capabilities of such assessments. It also demonstrates the potential of combining trade statistics, energy scenario analysis, and supply-chain mapping in the development of more informed and policy-relevant environmental evaluations of materials.

5 Conclusion

This doctoral work investigated the role of LCA in supporting the emerging SSbD framework, with a particular focus on the challenges and methodological adaptations needed to apply LCA effectively in early innovation phases and in the chemical sector. The research contributed both to the practical application of LCA within case studies and to the methodological development of tools and approaches required to meet the evolving demands of sustainability assessment under the SSbD initiative.

The first chapter presented a detailed application of the SSbD framework to a case study involving plasticisers used in food contact materials, demonstrating how LCA can support chemical substitution decisions by integrating technical performance, regulatory relevance, and environmental sustainability. The case study highlighted both the strengths and limitations of current LCA approaches in the SSbD context, especially where data availability or granularity is limited, and where functional equivalence must be carefully defined.

Building on these insights, the second chapter addressed the issue of comparability of chemicals in LCA, with a focus on intermediate products and how nomenclature systems and process classifications affect impact assessments. The analysis revealed that greater harmonisation and categorisation efforts are necessary to improve the interoperability of datasets and to ensure meaningful comparisons among chemicals and materials, particularly for regulatory or SSbD purposes.

In the third chapter, the thesis introduced a tool for rapid proxy building in the chemical sector, aimed at addressing the widespread lack of primary LCA data for many industrial chemicals. The tool leverages mass balance-based process mapping to reconstruct supply chains and generate plausible proxy datasets for environmental assessments. A realistic case study demonstrated the tool's capacity to trace upstream processes and identify key input substances, supporting LCA modelling in data-scarce contexts and enabling screening assessments for SSbD applications.

Finally, the fourth chapter explored the adaptation of existing LCA datasets to future scenarios, especially in terms of energy mix evolution within the European Union. By combining trade data with scenario-based energy inputs, the analysis provided a forward-looking assessment of plastics' environmental impacts under different decarbonisation pathways. This methodological advancement is crucial for SSbD evaluations, where future-ready technologies and supply chains need to be assessed for their prospective sustainability.

Overall, the contributions of this thesis lie in demonstrating both the applicability and the current limitations of LCA within the SSbD framework, using real-world case studies as practical validation (Chapter 1). Specific challenges identified during this application were further investigated to advance the state of knowledge (Chapter 2) and to support LCA practitioners through the development of dedicated tools (Chapter 3) and methodological approaches (Chapter 4).

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