Safe and Sustainable by Design Chemicals and Materials. Revised framework (2025)

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Contents

Abstract

The Safe and Sustainable by Design (SSbD) framework for chemicals and materials was developed by the European Commission Joint Research Centre (EC-JRC) in 2022, as the scientific basis for the European Commission Recommendation of 2022. The first version of the framework has since been tested in different contexts and by different stakeholders, providing a solid basis for the announced revision. The core concept of the SSbD framework is to **ensure safety and sustainability** throughout the entire life cycle of chemicals and products and to **steer innovation to design or redesign chemicals, materials, processes and products by identifying potential safety issues, sustainability impacts and trade-offs early-on.** The revised SSbD framework, presented here, maintains the core concept while introducing **novel aspects**:

1. **SSbD framework principles:** as the backbone of the framework, principles are listed to enhance clarity.
2. **Scoping analysis:** It is the process of identifying and prioritising the key issues associated with the intended innovation. The scoping analysis has been structured towards defining scenarios to tailor the application of the SSbD framework. The importance of engaging with the actors along the life cycle is emphasised. Methodological criteria are proposed to guide the SSbD practitioner to adhere to SSbD principles.
3. **New structure of the safety and sustainability assessment parts:**
    (a) The **safety** part is focused on the risks associated with the chemical/material and the related processes and uses. To this end, it combines the evaluation of the chemicals' intrinsic properties with that of occupational/professional, consumer, and environmental exposure. The Steps 1, 2 and 3 of the 2022 framework are now merged in one holistic safety part. To guide the selection of safer production processes and to enable a comprehensive evaluation of different pathways to produce the same chemical/material, there is a specific process-related safety sub-chapter.

    (b) The **environmental sustainability** part addresses the entire life cycle of the chemical/material (raw materials, production, use, and disposal process) and it is based on the application of Life Cycle Assessment. To simplify the SSbD application at low innovation maturity levels, this part proposes screening level assessments and LCA based benchmarks. To guide the selection of more sustainable production processes and to enable a comprehensive evaluation of different pathways to produce the same chemical/material, there is a specific process-related sustainability sub-chapter.

    (c) The **socio-economic sustainability assessment** part, which is significantly expanded compared with the 2022 framework, addresses the social fairness and competitiveness dimensions of the chemical/material supply chain. These include aspects related to supply chain vulnerabilities and life cycle costs, also linked to risk governance and financial stability.

4. **Evaluation**: this part illustrates an approach to evaluate the implementation of the SSbD framework, to identify trade-offs between the different safety and sustainability aspects and uncertainties of the assessment according to the available information. An example of visualisation of the results of the evaluation is provided as a **dashboard**, serving as a compass to identify hotspots and critical elements to guide the innovation along the life cycle of chemicals and materials.
5. **Documentation:** The framework also includes a chapter on documentation, aiming at systematically and transparently recording the key elements of the implementation of the SSbD approach.

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1. Introduction

Europe is the 2nd largest **chemical** producer in the world with sale of €650 billion in 2023. The chemical industry is the fourth largest manufacturing industry with 7% of EU manufacturing turnover, 1.2 million direct highly skilled jobs, with 3.6 million indirect jobs and 19 million jobs across all value and supply chains[1]. Moreover, the chemical industry is at the heart of many value chains: more than 50% of chemicals are sold to other industries. The sector is among the largest CO_2 emitters, as the global direct CO_2 emission from primary chemical production in 2022 equals 935 Mt[2].

Similarly, **materials** are a central element of the economy, and more and more are expected to be developed to respond to new competitiveness and technological challenges. For example, the European Commission's Communication on "Advanced Materials for Industrial Leadership," adopted in February 2024, outlines a strategy to position the EU as a global leader in advanced materials. Recognizing these materials as crucial enablers for the green and digital transitions, the Communication emphasises the importance of strengthening the EU's research, innovation, and production ecosystem.

Since its publication, the European Green Deal has been one of the priorities of the European Commission (EC). The European Green Deal aims to transform the EU's current economy into a greener and more sustainable one (EC, 2019). Within the Green Deal, the Chemicals Strategy for Sustainability (CSS) (EC, 2020a) identified several actions contributing to the reduction of negative impacts on human health and the environment associated with the production and use of chemicals, materials, products and services commercialised or imported in the EU. Among them, there are different actions to support innovation for safe and sustainable chemicals in the EU. The development of a framework to define safe and sustainable by design (SSbD) chemicals and materials can be considered as a key enabler for these actions.

In parallel, President Ursula von der Leyen, in preparation of her potential second term of mandate asked Mario Draghi to prepare a report on competitiveness of the European Union. The subsequent Competitiveness Compass transformed the recommendations of the Draghi report (Draghi, 2024), together with the conclusions of the Letta report (Letta, 2024) on the single market, into a roadmap.

The EU Competitiveness Compass outlines the strategic priorities for strengthening Europe’s industrial base. It is structured around three core pillars—innovation, decarbonisation, and economic security—alongside a set of cross-cutting enablers. This demonstrates that innovation is and will remain a fundamental pillar of the European Commission’s priorities, an ambition to which the revised SSbD framework strongly contributes, as illustrated in Figure 1.

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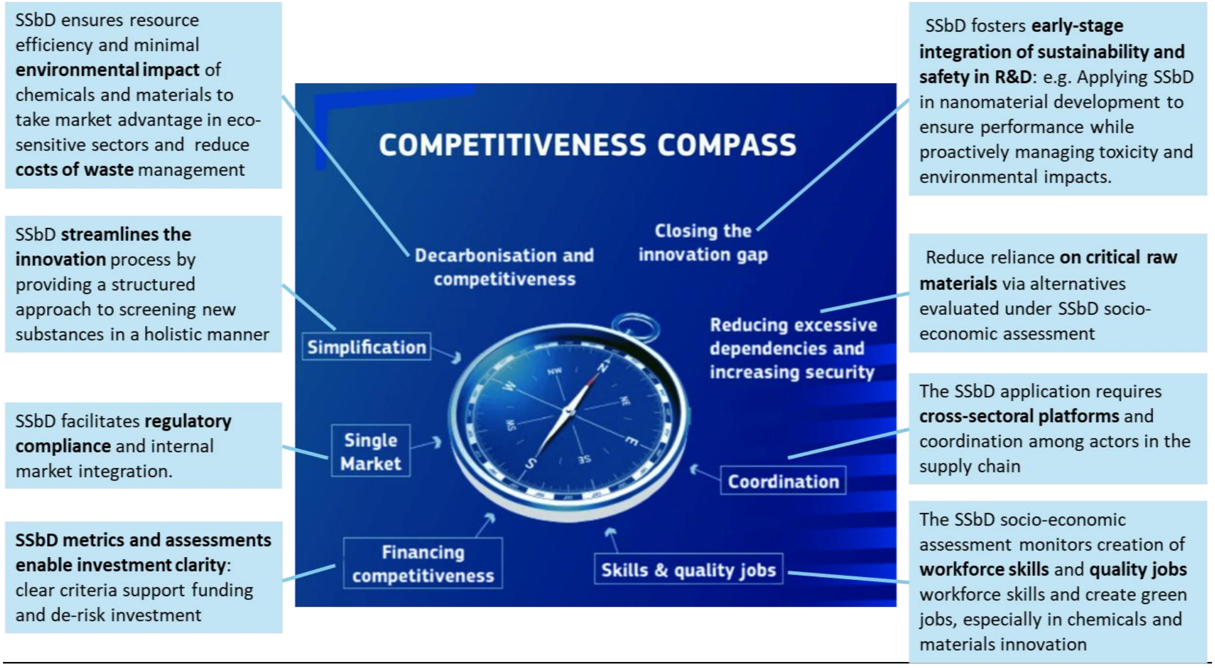
[1] As reported by CEFIC fact and figures of European chemical industry – 2024 (https://cefic.org/facts-and-figures-of-the-european-chemical-industry/)

[2] As reported by IEA (https://www.iea.org/energy-system/industry/chemicals)

Figure 1. Contributions of the SSbD framework to the EU industrial competitiveness.



SSbD ensures resource efficiency and minimal **environmental impact** of chemicals and materials to take market advantage in eco-sensitive sectors and reduce **costs of waste** management

SSbD **streamlines the innovation** process by providing a structured approach to screening new substances in a holistic manner

SSbD facilitates **regulatory compliance** and internal market integration.

SSbD metrics and assessments enable investment clarity: clear criteria support funding and de-risk investment

SSbD fosters **early-stage integration of sustainability and safety in R&D**: e.g. Applying SSbD in nanomaterial development to ensure performance while proactively managing toxicity and environmental impacts.

Reduce reliance **on critical raw materials** via alternatives evaluated under SSbD socio-economic assessment

The SSbD application requires **cross-sectoral platforms** and coordination among actors in the supply chain

The SSbD socio-economic assessment monitors creation of **workforce skills** and **quality jobs** workforce skills and create green jobs, especially in chemicals and materials innovation

Source: Own elaboration

The transition to safer and more sustainable chemicals/materials is a competitiveness driving concept which is increasingly recognised as a priority at global level, as reiterated also by the recent efforts on the Global Framework on Chemicals (UNEP, 2023), and the Stockholm declaration on chemistry for the future (*The Stockholm Declaration on Chemistry for the Future*, 2025).

Moreover, the recent Communication on the European Chemicals Industry Action Plan (EC, 2025), further supports strengthening the need for concrete measures, to secure the global competitiveness of the European chemicals industry, to maintain a strong European production base and to upgrade it. Among the actions, there are those related to alternative feedstocks (such as bio-based), to unlock secondary materials markets, and to identify options for reducing energy demand. The SSbD framework is expected to play an important role in driving the innovation of the chemical industry towards safer and overall, more efficient (from resources and environmental performance point of view) chemical industry.

The **purpose** of this report is to present a revised SSbD Framework that enhances its support for innovation while improving its relevance, reliability, and operability. The revised framework also considers the need for a simplified approach in the early stages of innovation, for Small and Medium-sized Enterprises (SMEs) and for companies first approaching the SSbD concept. **By integrating safety and sustainability from the earliest stages of innovation,** the **SSbD** framework can **support more resilient, competitive and innovation based, future-proof industrial ecosystems.**Since its publication in 2022, the SSbD Framework developed by the JRC (Caldeira et al., 2022b) has been tested in different applications and contexts. The Framework was first tested by the JRC in collaboration with industrial partners in three case studies (Caldeira et al., 2023). Subsequently, the Recommendation (EC, 2022) addressed to EU Member States, industry, academia, and research and technology organisations (RTOs) invited them to test the SSbD framework and provide feedback over a two-year testing period (Abbate et al, 2024; Garmendia et al, 2025). The aim of the testing was to gather information and gain experience to revise the Framework and improve its relevance, reliability and operability.

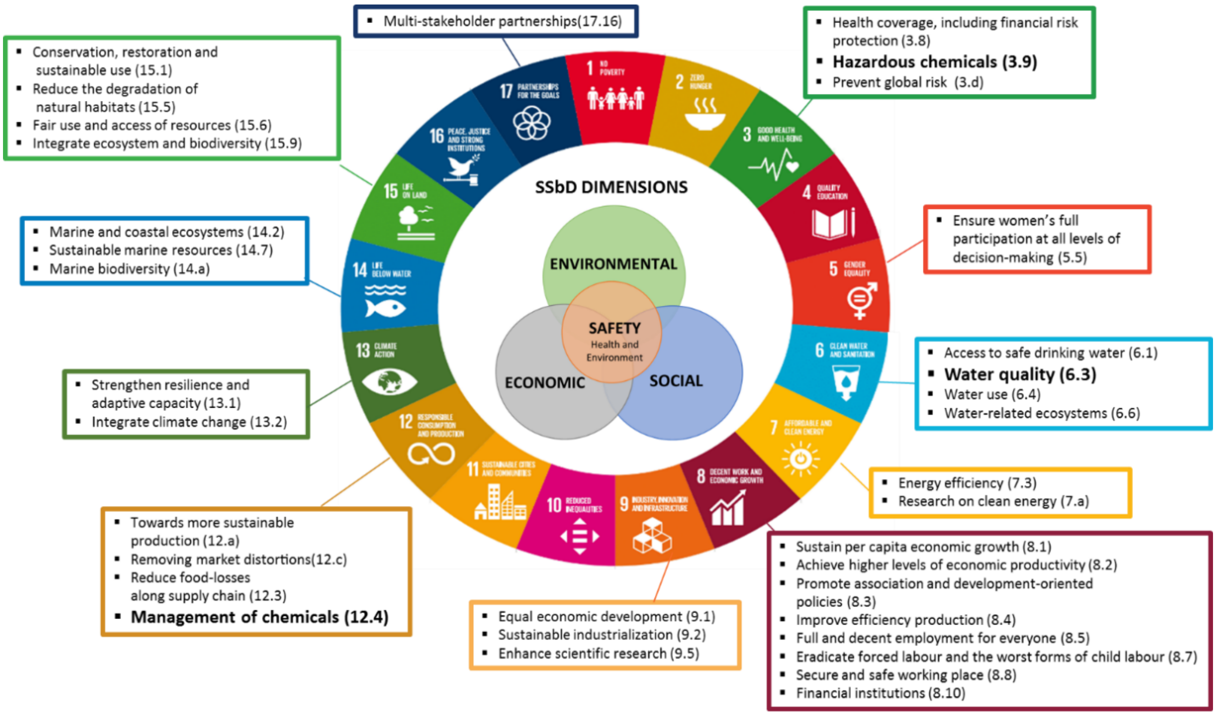
2. Background concepts

The concept of **sustainable development** came from the idea of reconciling economic growth with environmental limits and social justice. Defined in the Brundtland Report as meeting *"the needs of the present generations without compromising the ability of future generations to meet their own needs"* (WCED, 1987), it introduced the three sustainability pillars: economy, environment and society. This concept also forms the basis for the sustainability definitions outlined in ISO Guide 82:2019 (ISO, 2019).

The sustainability principles have been enunciated over time in various international documents, including the United Nations' **Sustainable Development Goals** (SDGs) outlined in the 2030 Agenda (UN, 2015). The 17 SDGs, including 169 targets and 231 indicators, cover the different dimensions of sustainability, providing principles and a reference for policy at different levels (local, national and regional level) and for business and corporate decision makers.

The transition towards SSbD chemicals and materials will contribute horizontally to several SDGs, especially SDG 3 Good Health and Wellbeing, SDG 12 Sustainable Consumption and Production, and SDG 6 Water Quality (UN, 2015). Figure 2 illustrates how the different aspects of the SSbD assessment are mapped against the SDGs, and its centre highlights that safety is an important aspect of the three sustainability pillars. While the safety and sustainability aspects are intrinsically linked, for ease of use, the framework addresses them separately.

Figure 2. Dimensions considered in the SSbD and related SDGs targets.



Source: Caldeira et al., 2022

To design safe(r) and environmentally (more) sustainable chemicals/materials, several principles have been proposed over time. The proposed principles are those considered in e.g. **green chemistry** (Anastas & Warner, 1998), **green engineering** (P. T. Anastas & Zimmerman, 2003), **sustainable chemistry** (Blum et al. 2017; ISC3, 2021; UBA, 2009; UNEP, 2021), **circular chemistry** (Keijer et al., 2019) and **safe by design** (OECD, 2020), as well as those linked to policy related ambitions (e.g. transition to a circular economy (EC, 2020b) or to a bioeconomy (EC, 2018a) and to zero pollution (EC, 2021a).

Many of these principles include both safety- and resources-related considerations. They intend to help the design or redesign of chemicals, materials and their related manufacturing processes and supply chains (Dekkers et al., 2020; Jantunen et al., 2021; OECD, 2020; Tavernaro et al., 2021), as well as their circularity aspects.

Another key concept underpinning the SSbD framework is **Responsible Research and Innovation** (Yaghmaei & Van De Poel, 2020). The Responsible Research and Innovation concept steers and manages innovation to connect the basic concerns of business with the global societal challenges. Moreover, it emphasizes the development of solutions to environmental and social problems through improved products, services, and business models (Halme & Korpela, 2014).

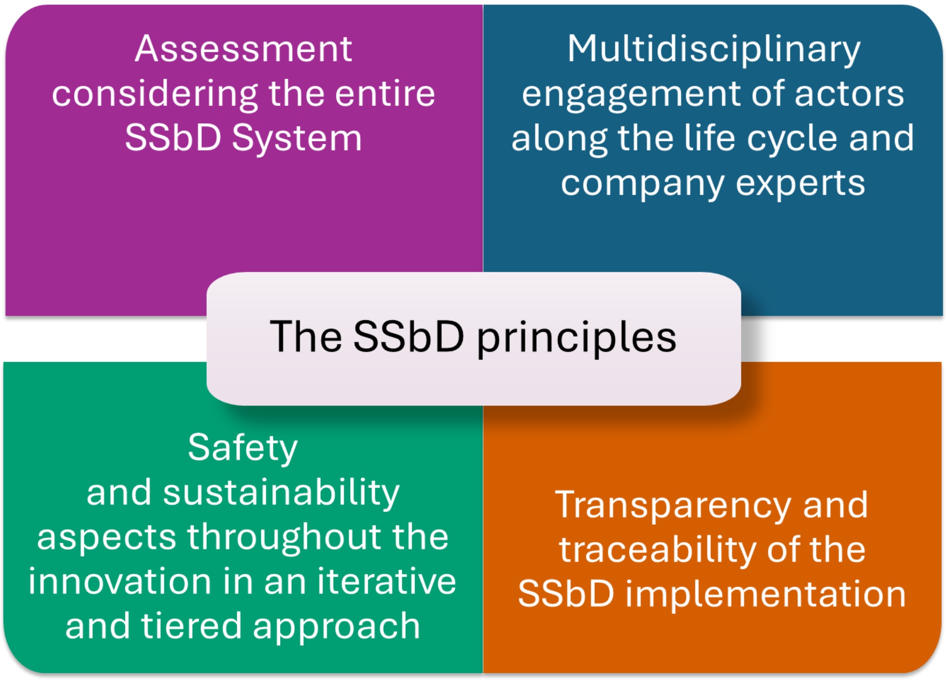
Finally, **Life Cycle Thinking (LCT)** is another key concept underpinning the SSbD framework. It aims to assess and consequently reduce emissions and resources use, as well as associated environmental impacts all along the entire life cycle of products - from raw material extraction to the end of life.

3. The SSbD principles

The SSbD framework serves as an approach to guide innovation towards safe and sustainable - or at least safer and more sustainable, as presently applied - chemicals and materials life cycles. The framework helps innovators to identify the necessary information to support safety and sustainability related decision-making, while minimising inherent uncertainties. **This framework is built on four SSbD principles** described below and shown in Figure 3.

- **Assessments consider the entire SSbD system** including chemicals /materials, processes and products under study and their related life cycles.
- **The SSbD concept builds on multidisciplinary engagement of the life cycle actors and company experts** to ensure that both safety and sustainability are considered throughout the entire innovation. It fosters collaboration to deliver the highest impact of the innovation type being considered, together with safety and sustainability performance.
- **Safety and sustainability aspects are addressed with a holistic perspective throughout the innovation**. The **iterative approach** in innovation also takes into consideration the inherent uncertainties and trade-offs in each iteration. SSbD is not static, but evolves over time, in function of new information on hazards and uses, new challenges and needs and new available innovative solutions. The **tiered approach** implies the gradual reduction of uncertainties by identifying information needs and gathering or generating data for each iteration, as the innovation process progresses.
- **The SSbD concept implies transparency of the assessment and traceability** of the fulfilment of the principles throughout the entire innovation.

Figure 3. SSbD framework principles.



Source: Own elaboration

4. Definitions and terms

The complete list with definitions and terms is provided in Annex 1.

- **By (re)design**: In the context of SSbD for chemicals and materials, the term ‘by-design’ can be interpreted as Molecular (re)design, Process (re)design, Product (re)design.
- **Chemical**: Substances and mixtures as defined in the Regulation (EC) No1907/2006 (EC, 2006) (hereafter, REACH).
- **Criteria**: Set of values (e.g. reference or class performance) on which a decision may be based.
- **Iterative approach:** At each innovation iteration SSbD is applied to the level of detail that can be achieved with the data and information available at that point in time. The SSbD structure is followed in each iteration.
- **Material:** Either substances or mixtures which may or may not yet fulfil the definition of an article under REACH and may be of natural or synthetic origin.
- **Maturity of the innovation:** will be defined and evaluated by the SSbD practitioner according to the used approach, for example Cooper stage-gate, Technological Readiness Level (TRL), low-medium-high or regulatory readiness level.
- **Maturity of SSbD:** While the maturity of the innovation will be defined and described by the SSbD practitioner according to different criteria, the maturity of the SSbD implementation reflects the completeness of the fulfilment of the SSbD principles: simplified, intermediate or full.
- **Methodological criteria:** set of structured conditions to support building from one SSbD scenario to another to fulfil the SSbD principles and full SSbD implementation.
- **Mixture**: is defined in REACH as a mixture or solution composed of two or more substances.

- **Process:** series of interconnected steps or operations (chemical and physical transformations) that take place between the raw materials extraction and the finished product, or that transform one type of material into another, including its End of Life (EoL).
- **Product:** Any good or service which is supplied for distribution, consumption or use. Definition adjusted from EU Ecolabel (EC, 2010).
- **SSbD practitioner:** Refers to any individual or group of professionals from the diverse disciplines required to implement the Safe and Sustainable by Design (SSbD) approach (e.g., innovators, chemists, toxicologists, materials scientists, engineers, sustainability experts). An SSbD practitioner is a professional who, regardless of their specific technical background, is capable of adopting a holistic and systems-oriented perspective on innovation—integrating safety, sustainability, and functionality considerations across the entire life cycle of a chemical, material, or product.
- **SSbD system:** skeleton of the system under assessment, including chemicals/materials, processes, and products and their related life cycles according to the intended innovation.
- **SSbD scenario:** the specific and real set of conditions (scoping analysis elements) that define the context in which the SSbD assessment is carried out.
- **Substance**: a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition.
- **Tiered approach**: approach built on a gradually increasing amount and quality of data generated and collected as the innovation progresses in the SSbD implementation.

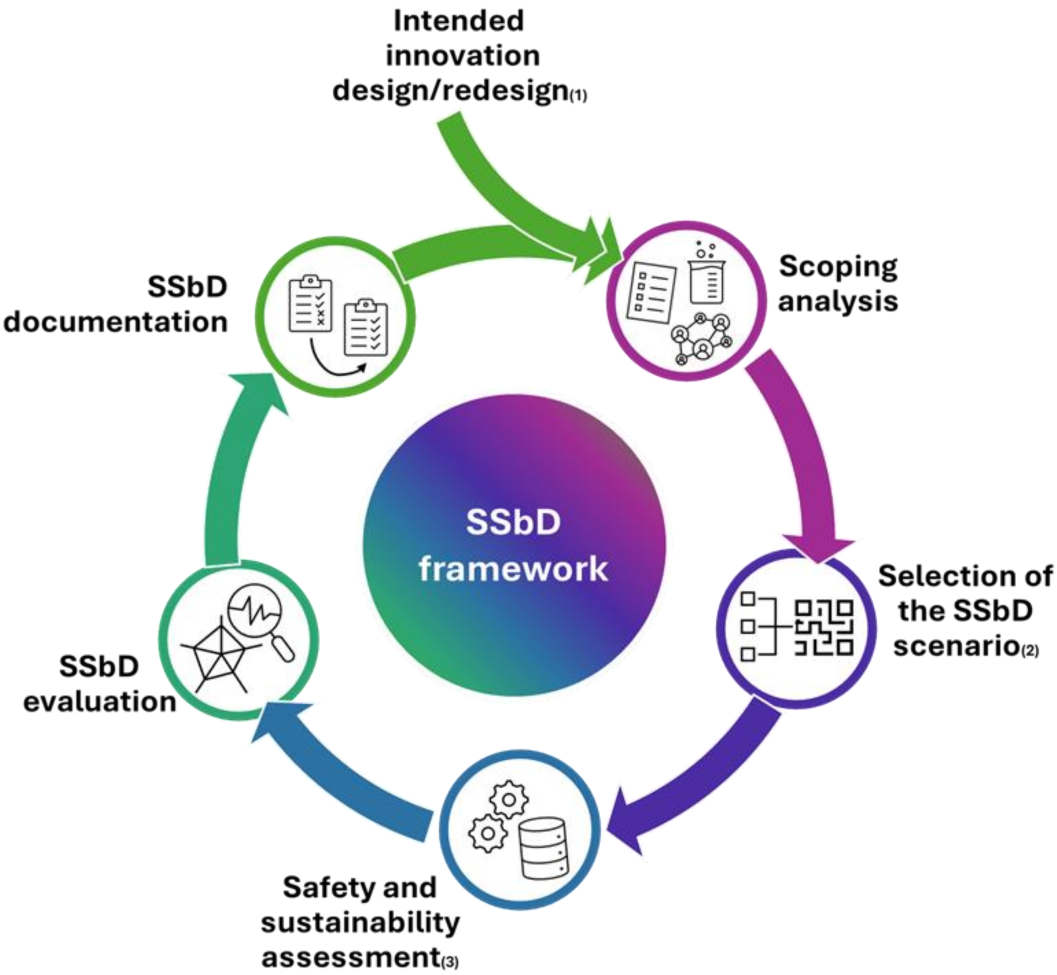
5. Overall structure of the SSbD framework

The circular structure of the SSbD framework emphasises the iterative nature of its implementation throughout the innovation process. Below is a brief description of all the components, with detailed explanations provided in the following chapters.

- **Intended innovation – design/redesign:** The aim of the SSbD is to guide chemicals and materials innovation from the (re)design, along all the innovation stages, scaling up from prototyping, to market readiness. Assessing the innovation in terms of its capacity of delivering safer and more sustainable solutions the SSbD acts as a compass throughout the innovation process, since **applying design principles** (Annex 3) **in the (re)design phase alone is not enough. To ensure safety and sustainability it is essential to perform an assessment as means to unveil hotspots and trade-offs, to be addressed during the innovation.**
- **Scoping analysis (Chapter 6)**: defines the objectives, principles and decision rules of the intended innovation. It includes the description of the initial SSbD system under study, the contextualization of the intended innovation, including the (re)design, and identification of the actors along the life cycle.
- **SSbD scenario (Chapter 7)**: represents the outcome from the scoping analysis and identifies the entry point to the SSbD assessment, which allows to tailor the safety and sustainability assessments accordingly.
- **Safety and Sustainability assessment (from Chapter 8 to Chapter 11.3)**: includes the holistic assessment of safety and sustainability aspects along the entire life cycle of the chemical/material, for both environmental and socio-economic aspects.
- **SSbD evaluation (Chapter 13)**: presents the outcome of the safety and sustainability assessment, and compares the results in an iterative manner with the objectives, principles and decision rules defined in the scoping analysis. A proposal for visualizing the results in a dashboard is proposed.
- **Documentation (Chapter 14):** proposes a possible template for recording the implementation of the SSbD Framework in a traceable and transparent manner, outlining the actions and objectives for the subsequent iteration.

The overall structure of the SSbD framework is shown in Figure 4 below.

Figure 4. Overall structure of the SSbD framework.



(1) Innovations can be triggered for example by the need of improving existing portfolios, new market/consumer requests, new ambitions and priorities and/or policy priorities

(2) Key moment where the tailored safety and sustainability assessment is defined according to the outcomes of the scoping analysis

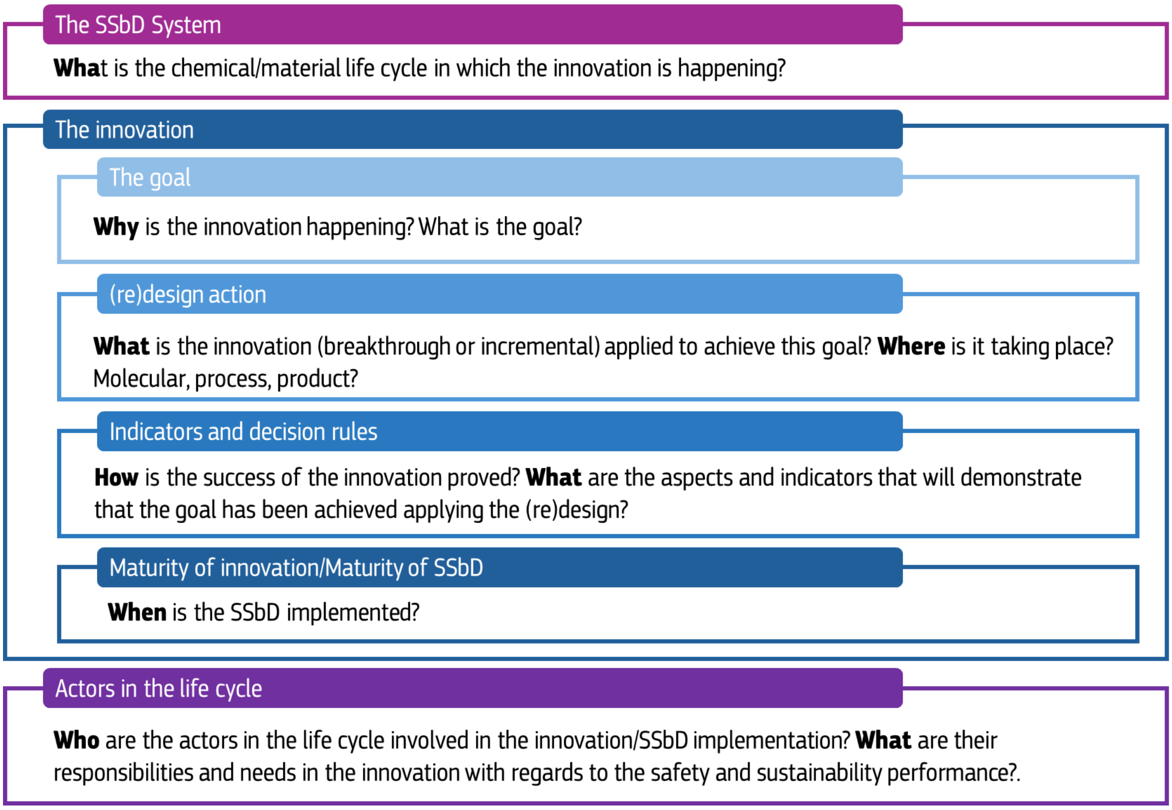
(3) The safety and sustainability assessment are tailored based on the *selected SSbD scenario*

Source: Own elaboration

6. Scoping analysis

This section frames the intended innovation (6.1) as an entry point to the SSbD. The scoping analysis contextualises the intended innovation to which the SSbD framework will be applied. Figure 5 summarises the elements of the scoping analysis that rationalises the SSbD prior to proceeding with the safety and sustainability assessment.

Figure 5. Elements of the scoping analysis.



The SSbD System

What is the chemical/material life cycle in which the innovation is happening?

The innovation

The goal

Why is the innovation happening? What is the goal?

(re)design action

What is the innovation (breakthrough or incremental) applied to achieve this goal? **Where** is it taking place? Molecular, process, product?

Indicators and decision rules

How is the success of the innovation proved? **What** are the aspects and indicators that will demonstrate that the goal has been achieved applying the (re)design?

Maturity of innovation/Maturity of SSbD

When is the SSbD implemented?

Actors in the life cycle

Who are the actors in the life cycle involved in the innovation/SSbD implementation? **What** are their responsibilities and needs in the innovation with regards to the safety and sustainability performance?.

Source: Own elaboration

The scoping analysis includes:

- The description of the initial SSbD system under study (6.2),
- The description of the intended innovation – including design principles that can guide the innovation (6.3)
- Engagement with the actors along the life cycle to obtain a complete set of information on the SSbD system (6.4).

The three building blocks are necessary, but their implementation order depends on the actual case.

6.1. Intended innovation

The SSbD framework is intended for any organisation innovating in the context of chemical/materials and their life cycles. Furthermore, by linking the SSbD framework principles with the innovation strategy and management, organisations may build a governance model that inherently values safety and sustainable practices and align their innovation strategy with broader objectives such as regulatory compliance, market differentiation or responsible resource use (Stoycheva et al., 2025).

Innovations can be triggered for example by the need of improving existing portfolios, new market/consumer requests, new ambitions and priorities and/or policy priorities (Figure 6).

The alignment of the innovation strategy and management with SSbD ensures that safety and sustainability considerations are embedded in every strategic decision. The application of the SSbD framework should not only reduce the likelihood of costly missteps, resource use, accidents, regrettable substitutions of chemicals, processes or materials, but should also position the company as a leader in responsible innovation and related innovation in the use of data systems – including supply/downstream stages - and facilitate fast compliance, with the associated “fist mover” competitive advantages, where relevant to the level of innovation being proposed.

The SSbD framework can be applied to:

- Existing cases or systems (e.g. existing portfolios) to check and assess safety and sustainability performance (according to the EC SSbD Framework). The goal in these cases can be the identification of information and data gaps or the prioritisation of the chemical/material for innovation in a portfolio.
- Innovations that can be:
  - Incremental innovations, consisting of continuous enhancements and refinements of any of the aspects (e.g. functionality, process efficiency, safety, sustainability etc) of existing chemicals, materials, products, services, or processes
  - Disruptive/breakthrough innovations, introducing ground-breaking solutions, challenging existing market norms and creating new value propositions.

Figure 6. Definition of the innovation in the context of SSbD.

What is the general type of the innovation?

It might be a truly novel solution, i.e. a breaktrough or game-changing innovation, but in most cases, it would be an improvement of an existing solution, i.e. incremental.

What is the goal of the innovation?

The goal could be related to safety, sustainability but also the functionality or other aspects in the SSbD system

Why is SSbD applied?

To ensure the overall safety and sustainability performance of an existing or new system.
To demonstrate that safety and sustainability is improved in a life cycle thanks to an innovation.

Source: Own elaboration

6.2. Definition of the system under study

The definition of the SSbD system under study includes the chemicals/materials, processes and products under study, and their related life cycles according to the intended innovation (Box 1).

Box 1. Consideration of life cycles to define the SSbD system.

Substances, mixtures, materials, and products form a nested, interdependent hierarchy within industrial value chains. A substance is the basic chemical entity. Substances are combined to form mixtures or transformed into materials with specific structures and functions. These mixtures and materials are then incorporated into products, which deliver the final service to users.

Because each level builds on the previous one, their life cycles are intrinsically interconnected. The life cycle of a substance—covering synthesis, formulation, use, and waste—feeds directly into the life cycle of the mixture or material in which it is used. In turn, the life cycle of a product incorporates the life cycles of all materials and substances from which it is composed.

Mixtures and materials may be addressed within the substance life cycle (e.g. during formulation or as a product), yet they may also be assigned distinct life cycles, as their intrinsic properties—and consequently their safety considerations—are specific to their own chemical, physical and structural characteristics.

This creates a complex system in which decisions made at the substance level can influence performance, safety, sustainability, and end-of-life behaviour at the material and product levels. Likewise, product design and use conditions can determine how substances behave, are released, or can be recovered.

Moreover, the interplay across these levels—combined with diverse value chains, multiple actors, and numerous transformation steps—means that addressing safety and sustainability requires a system-wide perspective, rather than treating substances, materials, and products in isolation.

Life cycle stages in the SSbD system

Source: Own elaboration

The starting point of the definition of the system to be assessed will depend on the practitioner's position in the life cycle. **The SSbD system should always cover the three elements (chemical(s)/material(s), process(es) and product(s)) that are needed to define the boundaries for the assessment.**

The key elements for the definition are listed in Table 1**,** while examples of possible compilation of the scoping analysis are provided in Annex 2 of the document.

Table 1. Key elements for the definition of the system under study.

Identification of	Why it is needed	What should the SSbD practitioner consider
Chemical/ material	The definition of the chemical/material is fundamental in order to define the SSbD system as the rest of the elements will be linked to it. The identification and characterisation of the chemical/material is key as its intrinsic properties are determinant for both safety and sustainability assessment. The identification of the chemical/material will also support the identification of the processes and products of which it is a part and in which its intrinsic properties will have an impact.	▪ Chemical/material identification: Molecular structure, composition, identifier…. ▪ Physico-chemical properties: molecular weight, solubility, pH, boiling/melting point, vapor pressure, partition coefficient, and reactivity…. ▪ Purity and impurities: main components and impurities, additives, stabilisers… ▪ Morphology and structure: particle size, shape, surface area, crystal structure…. ▪ Stability and transformation: changes under relevant environmental or biological conditions (e.g. oxidation, degradation, dissolution).
Process(es)	While the intrinsic properties of the chemical/material remain unchanged during the entire life cycle, the impact of the chemical/material will be specific to how it is used and manufactured. Identifying the raw material extraction, any further processing and end of life, the SSbD practitioner will be able to assess the chemical/material impact to the exposed humans and/or environment in these activities.	▪ Activities of the first actor in the life cycle of a chemical/material, the manufacturer/producer of the chemical/material, and includes processes by which the chemical/material is produced from raw materials. ▪ Processing activities like formulation where relevant, and/or other activities undertaken by workers. ▪ Processing of semi-finished products with the aim of producing the final product (e.g. calendering, spraying, extrusion). ▪ Activities related to the End of Life (waste disposal or recovery) are also considered.
Product/ application(s)	The identification of the final product/application enables the assessor to explore how the chemical/material is used and also assists the understanding of the role/impact of the chemical/material in the safety, sustainability and functionality in the end product and application, notably for the population using the product and being exposed to it.	▪ The identification of the industry sector and type of product, as well as the function (or service) that the chemical/material provides to the product/application. ▪ Regulatory requirements related to safety and functionality performance that the product/application must fulfil for the innovation to be placed on the market.

Source: Own elaboration adapted from Abbate et al., 2024

6.3. Description of the intended innovation and design principles

The description of the innovation includes information such as the goal(s) of innovation, the type of innovation (see chapter 5), and the nature of the (re)design. Moreover, whenever possible, during this phase the SSbD practitioner may also define decision rules and uncertainty aspects for the later stage of the evaluation. See chapter 13 for a comprehensive description of the decision-making rules and evaluation procedure.

Goals should reflect why the SSbD is applied e.g. what safety and sustainability aspects are driving the organisation to innovate. The nature of the (re)design will identify the specific actions (e.g. indicators, design principles etc.) toward the achievement of these goals and the decision rules will identify the indicators to measure the success of the action towards achieving these goals.

The SSbD framework covers (re)design activities comprising:

- Molecular design: the design of new chemicals and materials based on the atomic level description of the molecular system. This type of design effectively delivers new substances, whose properties may, in principle, be tuned to deliver specific functionalities and/or to be safe(r) and (more) sustainable.
- Process design: the design of new or improved processes to produce and process chemicals and materials. Process design does not change the intrinsic properties (e.g. hazard properties) of the chemical or material, but it can make the production of the substance safer and more sustainable (e.g. more energy or resource efficient production process, minimising the use of hazardous substances in the process). The process design includes upstream steps, such as the selection of the feedstock.
- Product design: the design of the product in which the chemical/material might be used with a specific function that will eventually be used by industrial workers, professionals or consumers.

In the scoping analysis, it is important to take into consideration that, depending on the nature of (re)design, one or more life cycle stages could be affected. Thus, the importance is thus stressed of the engagement with actors along all the life cycle stages.

The decision rules and the indicators measure the success of the action towards achieving these goals. In addition, decision rules will take into consideration aspects like uncertainties related to the assessment of these and other indicators. They will set the basis for the decision making during the evaluation by defining for example quantitative or qualitative criteria for the relevant aspects and/or indicators as well as weighting rules.

Design principles to guide safer and more sustainable innovation

Design principles can guide innovation by defining specific goals, the nature of the (re)design action applied (Table 2) and an example of the indicators to measure the success of the action towards achieving these goals (Table 3).

These design principles mainly include safety and resource related aspects during the process, as well as circularity aspects through EoL consideration. Once applied in the innovation process, the assessment of safety and sustainability assessment should ensure the proposed innovation is safer and more sustainable.

Table 2. Some SSbD design principles and associated definitions, and examples of actions and indicators that can be used in the design phase (table terminology explained below).

SSbD principle (based on)	Definition
SSbD1 Material efficiency (GC2, CC2, GC8, GC9, GC5, CC5, GC1, SC2)	Pursuing the incorporation of all the chemicals/materials used in a process into the final product or full recovery inside the process, thereby reducing the use of raw materials and the generation of waste.
SSbD2 Minimise the use of hazardous chemicals/materials (GC3, SC1, GR1, GC4, GE1, GR3, GC5)	Preserve functionality of products while reducing or avoiding the use of hazardous chemicals/materials where possible.
SSbD3 Design for energy efficiency (GC6, CC4, GE4, GE5, CC8, GE8, GE10, GE3, GR7, GC8, GC9, CC10)	Minimise the overall energy used to produce a chemical/material in the manufacturing process and/or along the supply chain.
SSbD4 Use renewable sources (GC7, CC3, GE12, SC2)	Target resource conservation, either via resource closed loops or using renewable material / secondary material and energy sources.
SSbD5 Prevent and avoid hazardous emissions (GE11, GC11, CC6, SC2)	Apply technologies to minimise and/or to avoid emission of hazardous pollutants into the environment.
SSbD6 Reduce exposure to hazardous substances (GC12, GR4, SC1)	Reduce or eliminate exposure to chemical/material hazards from processes as much as possible. Chemicals/materials which require a high degree of risk management should be avoided where possible and the best technology should be used to avoid exposure along all the life cycle stages.
SSbD7 Design for end-of-life (GC10, CC1, CC7, GE11, CC9, GE9, GE6, GE7)	Design chemicals/materials in a way that, once they have fulfilled their function, they break down into products that do not pose any risk to the environment/humans. Design for preventing the hindrance of reuse, waste collection, sorting and recycling/upcycling. Design to promote circularity.
SSbD8 Consider the whole life cycle (GE6, GR2, SC3, GR6, GR8)	Apply the other design principles thinking through the entire life cycle, from supply chain of raw materials to the end-of-life in the final product
SSbD9 Ensure responsible sourcing and minimise social risks	Avoid that procurements are linked with severe human rights and labour rights abuses, as well as other unethical practices. Perform a suppliers' assessment based on social performance and risk. Include ESG performance as a criterion for suppliers' selection Scrutinise suppliers operating in conflict-affected and high-risk areas

GC: Green Chemistry Principle, GE: Green Engineering Principles, SC: Sustainability Chemistry Criteria, GR: UBA Golden Rule, CC: Circularity Chemistry Principles.

Source: Own elaboration adapted from Caldeira et al 2022b

These design principles build upon those developed in different contexts, e.g. in green chemistry (GC) (P.T. Anastas & Warner, 1998), green engineering (GE) (P. T. Anastas & Zimmerman, 2003), circular chemistry (CC) (Keijer et al., 2019), the Golden Rules (GR) developed in UBA (German Environment Agency, 2016) , sustainable chemistry (SC) (UBA, 2009), and safe by design (OECD, 2020) as well as policy related ambitions (e.g. transition to a circular economy (EC, 2020b), to a bio-economy (EC, 2018), to zero pollution (EC, 2021a) etc.).

Table 3. Example on how design principles define the specific goal, (re)design action and indicators and decision rule/criteria.

SSbD principle (based on)	**Goal**	**(re)design actions**	**Indicator**	**Decision rule/criteria**
Use renewable sources **(GC, CC, GE, SC)**	Target resource conservation, either via resource closed loops or using renewable material / secondary material and energy sources.	Verify the possibility of selecting feedstocks that: - are renewables or secondary materials - do not create land competition and / or processes that: - use energy resources which are renewable and with low carbon emissions	- Renewable or fossil feedstock? (yes/no) - Recycled content (%) - Share of Renewable Energy (%)	Decision rule: the 3 criteria must be me: - Yes - No - 15%-30%

Source: from Caldeira et al 2022b

The list is illustrative and not exhaustive. The design principles goals, actions, and indicators are presented in Annex 3. They can be adapted by the developers to suit their innovation purposes.

6.4. Engagement with the actors along the life cycle

The scoping analysis helps to understand the position of an organisation in the life cycle and assists in identifying and engaging with actors/stakeholders along the life cycle early in the R&I process.

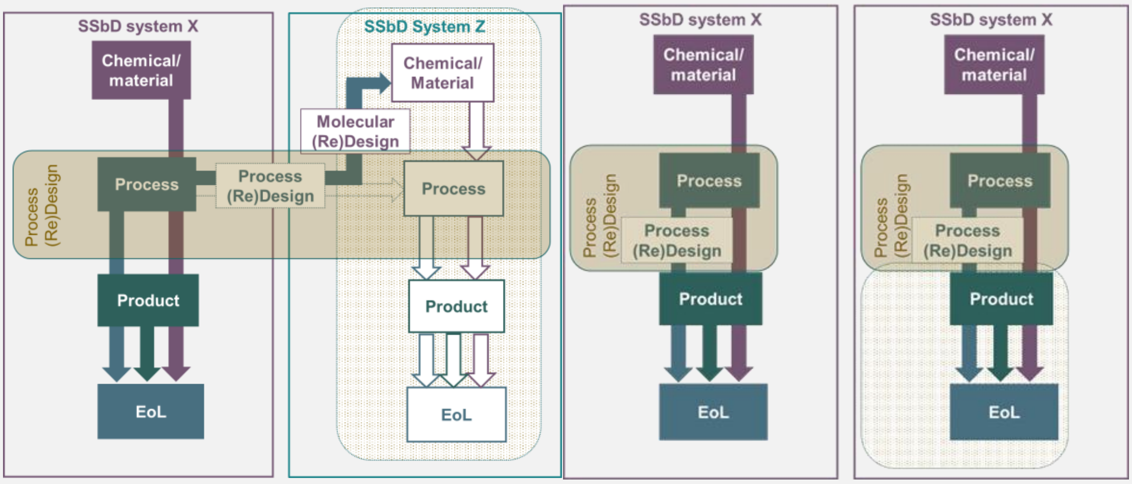
The SSbD framework goes beyond a single stakeholder and envisages the involvement and collaboration of stakeholders along the life cycle. All the actors involved in the life cycle of a chemical/material have a role in ensuring that the chemical/material, process, and product is safe, sustainable, and functional (Figure 7).

The engagement with life cycle actors also contributes to a better understanding on the technical and legal requirements related to the proposed innovative solutions. The SSbD practitioner may consider these requirements in the decision rules in order not to jeopardise the product's successful entry in the market at the end of the innovation. Chapter 14 provides a checklist on how to engage with stakeholders along the life cycle to collect the needed information for the scoping analysis. Further explanation regarding the engagement with the life cycle is provided in section 3.5.2 of the Methodological guidance (Abbate et al., 2024). Additional considerations are reported in Box 2.

Box 2. Consideration of direct and indirect consequences of (re)design action in the SSbD system.

Ideally engagement with actors in the life cycle would help to understand the SSbD system to the detail is needed and to understand the potential consequences of the (re)design in this entire SSbD system.

Depending on the nature of (re)design, one or more SSbD systems could take part of the innovation. Moreover, the SSbD practitioner should bear in mind that depending on the type of nature of the (re)design, this can have direct or indirect consequences in the overall life cycle safety and sustainability performance.



Source: Own elaboration

However, in most of the cases the implementation of the SSbD starts with a single actor in the value chain innovating.

The methodological criteria (Figure 7 and Figure 9) build on the different potential scenarios and provides guidance on how to reach the goal according to the SSbD principles.

7. Identification of the SSbD scenario

The SSbD scenario represents the outcomes from the scoping analysis that define the context in which the SSbD assessment is carried out. SSbD assessment should be understood as the fulfilment of the SSbD principles (simplified, intermediate or full SSbD). The SSbD scenario is built based on the scenarios identified for each of the elements of the scoping analysis summarised in Table 4. The outcome of the scoping analysis will define the entry point (in the first iteration) to the SSbD implementation. The following iterations of the scoping will reflect the progress in the fulfilment of the SSbD principles and define the new scenario for the next iteration.

Table 4. Example of possible scenarios identified for each of the elements of the scoping analysis and building on the fulfilment of the SSbD framework principles[3].

SSbD System	Innovation	Actors in life cycle	Link with the documentation (Chapter 14)
Simplified SSbD system: One element of the system is defined to the detail and certainty (reality) needed. while others remain generic and conservative	**Single innovation:** The innovation will be limited to the specific life cycle stage (element of the SSbD system) in which the innovation takes place.	**Single SSbD practitioner:** The SSbD implementation will be limited to the specific life cycle stage of the SSbD practitioner.	**Simplified SSbD:** Through the scoping analysis the SSbD practitioner will define the scenario applicable to the SSbD and the starting point of the SSbD implementation.
Intermediate SSbD system: Some elements of the system will be defined to the detail and certainty (reality) that is possible while others remain generic and conservative	**Collaborative innovation:** This initial innovation might affect near life cycle stages and trigger innovation considerations upstream and downstream.	**Collaboration SSbD practitioner:** The SSbD implementation will be a collaboration of several life cycle actors.	**Intermediate SSbD:** In each iteration of the implementation of the SSbD the new knowledge acquired in the previous iteration will be added to the new one. This will serve to refine the scoping analysis, to then define the new scenario.
Full SSbD system: The whole SSbD system is defined to the detail and certainty (reality) that is possible	**Full life cycle innovation:** Full life cycle innovations are considered. Safety and sustainability performance of the full SSbD system is ensured.	**Full SSbD practitioner:** As far as possible all life cycle actors are engaged and contribute to the overall SSbD implementation.	**Full SSbD:** At the end of the innovation the documentation should illustrate the progress in the SSbD implementation throughout the different iterations of the SSbD.

Source: Own elaboration

Methodological criteria are a set of **structured conditions** to support building from one scenario to another to fulfil the SSbD principles. Figure 7 provides an illustrative example on how the implementation of the SSbD can start with a single actor in the value chain innovating on a specific stage of the life cycle. However, to fulfil the SSbD principles the methodological criteria guide towards the consideration and engagement with all actors in the life cycle.

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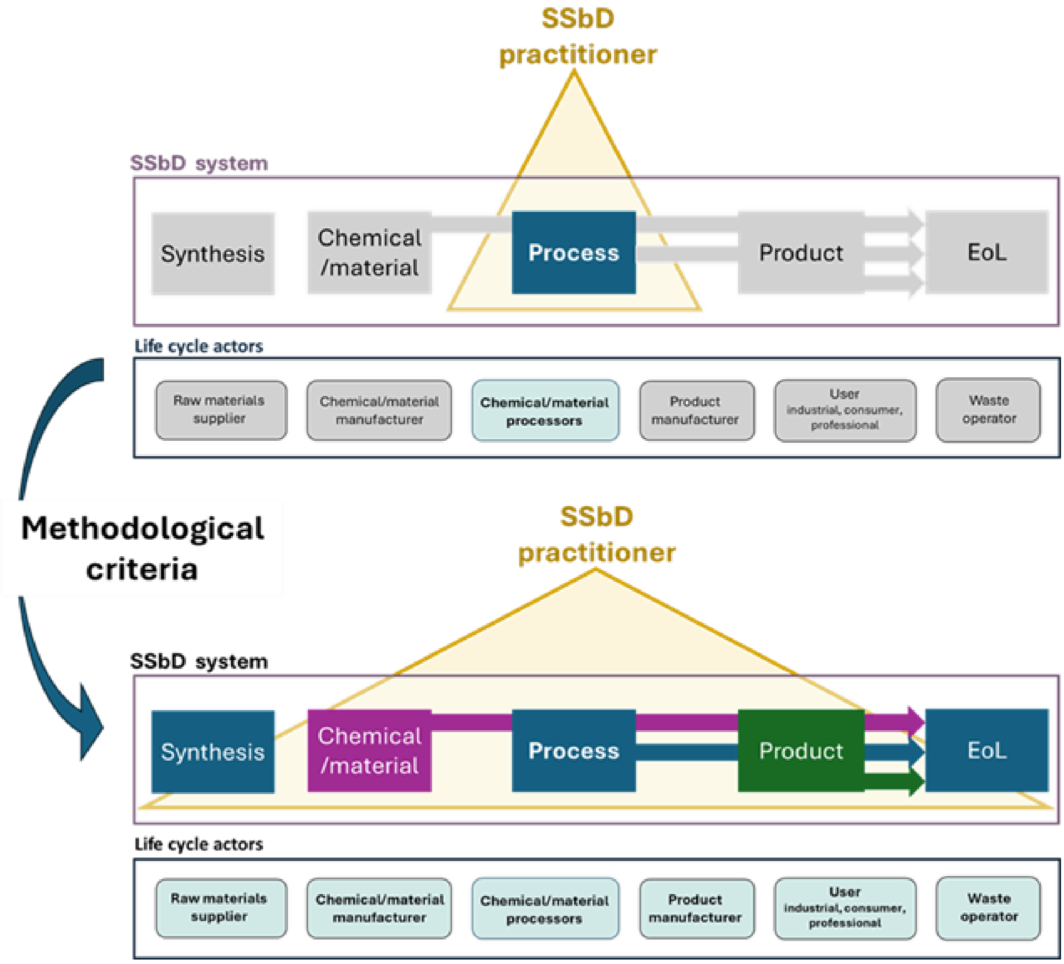
[3] This table aims to illustrate examples of the scoping analysis elements that will result in simplified, intermediate or full SSbD principles completeness. It is, by no means, exhaustive.

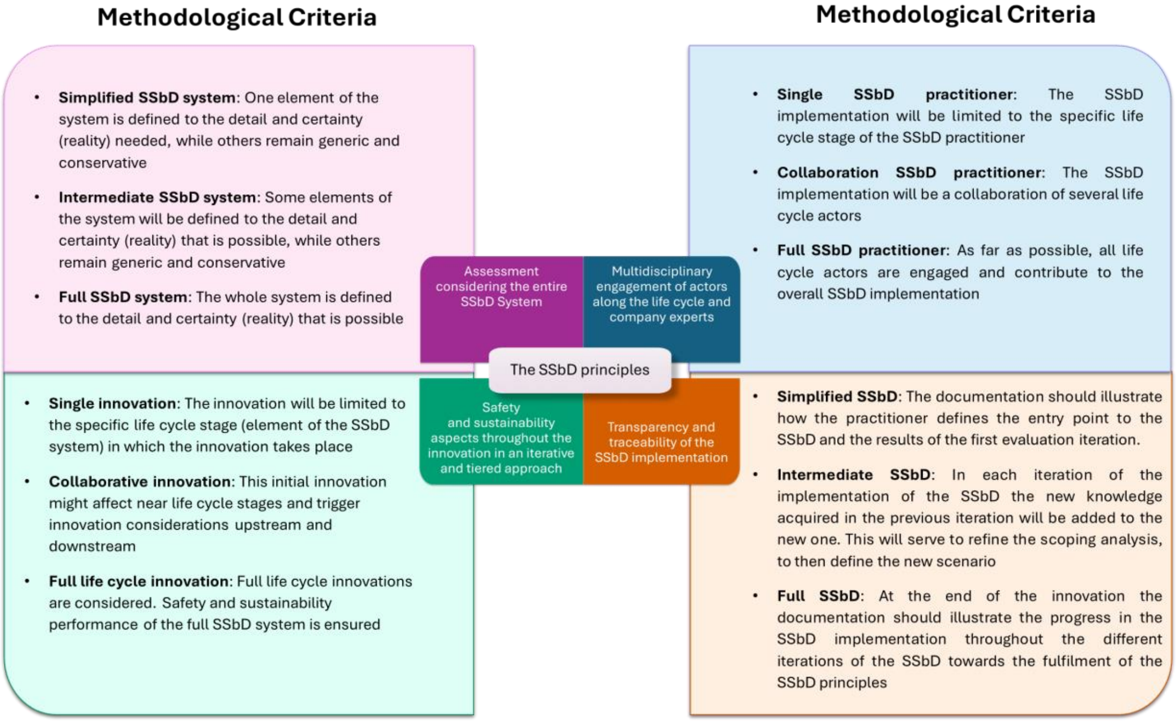
Figure 7. Types of actors involved along the life cycle.



Source: Own elaboration

Methodological criteria accompany the evolution of the SSbD scenario towards a full SSbD assessment (Figure 8).

Figure 8. Methodological criteria addressing SSbD principles.



- **Simplified SSbD system**: One element of the system is defined to the detail and certainty (reality) needed, while others remain generic and conservative
- **Intermediate SSbD system**: Some elements of the system will be defined to the detail and certainty (reality) that is possible, while others remain generic and conservative
- **Full SSbD system**: The whole system is defined to the detail and certainty (reality) that is possible

- **Single SSbD practitioner**: The SSbD implementation will be limited to the specific life cycle stage of the SSbD practitioner
- **Collaboration SSbD practitioner**: The SSbD implementation will be a collaboration of several life cycle actors
- **Full SSbD practitioner**: As far as possible, all life cycle actors are engaged and contribute to the overall SSbD implementation

- **Single innovation**: The innovation will be limited to the specific life cycle stage (element of the SSbD system) in which the innovation takes place
- **Collaborative innovation**: This initial innovation might affect near life cycle stages and trigger innovation considerations upstream and downstream
- **Full life cycle innovation**: Full life cycle innovations are considered. Safety and sustainability performance of the full SSbD system is ensured

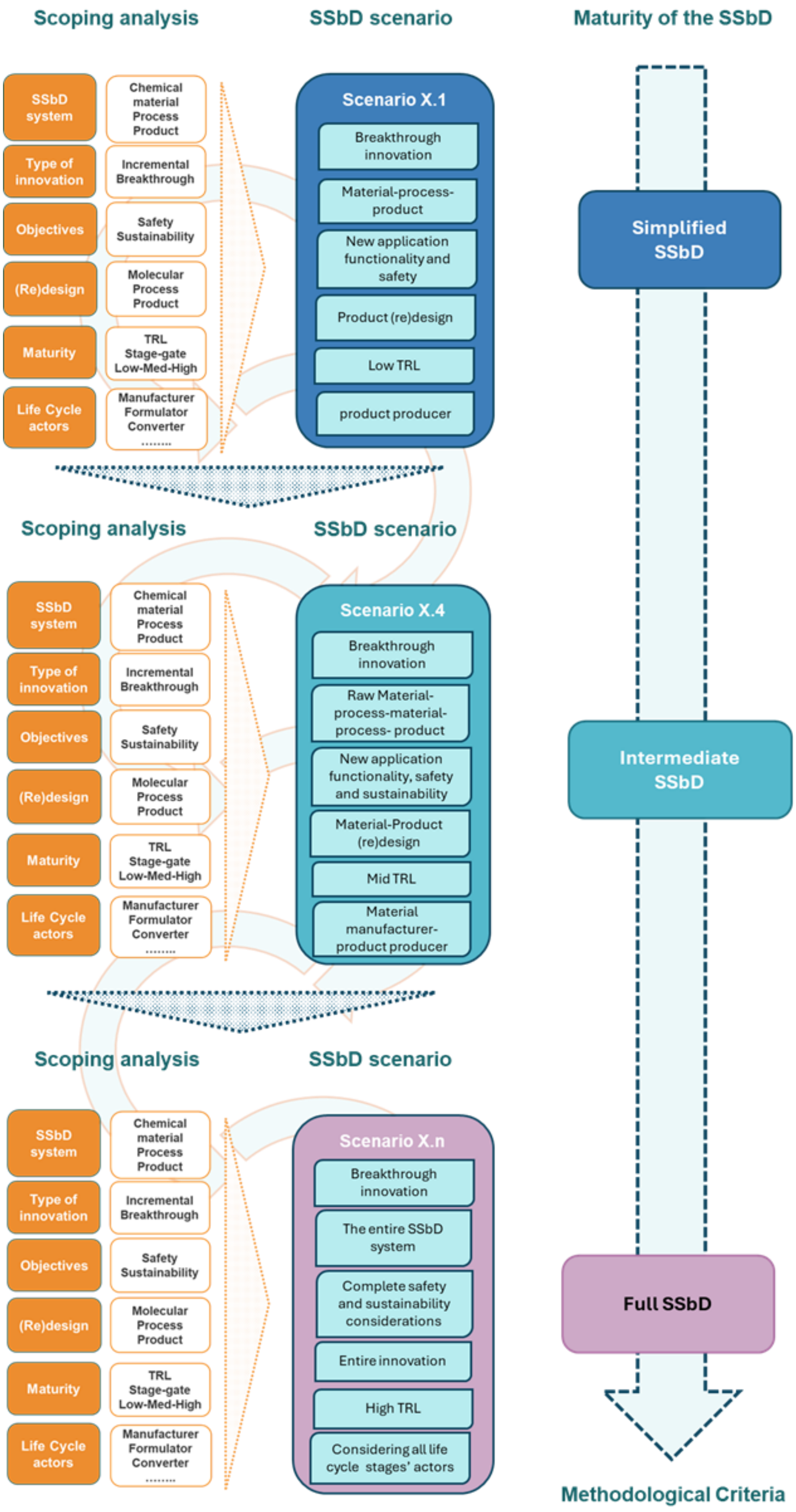
- **Simplified SSbD**: The documentation should illustrate how the practitioner defines the entry point to the SSbD and the results of the first evaluation iteration.
- **Intermediate SSbD**: In each iteration of the implementation of the SSbD the new knowledge acquired in the previous iteration will be added to the new one. This will serve to refine the scoping analysis, to then define the new scenario
- **Full SSbD**: At the end of the innovation the documentation should illustrate the progress in the SSbD implementation throughout the different iterations of the SSbD towards the fulfilment of the SSbD principles

Source: Own elaboration

The more advanced the innovation, the greater the understanding and certainty will be with regard to the scenario and the safety and sustainability data and quality.

Figure 9 provides a flow chart illustrating how the different elements of the scoping analysis support the SSbD practitioner in identifying the scenario and thus the entry point to the assessment. It also illustrates how the methodological criteria accompany the evolution of the assessment towards a full SSbD implementation.

Figure 9. Flow chart illustrating how the outcomes of the scoping analysis feed into the definition of the specific scenario.



The figure also illustrates how the methodological criteria accompany the evolution towards a full SSbD implementation. Several SSbD aspects (safety and sustainability assessment, SSbD evaluation and documentation), which are not included in this figure, are addressed between the different scoping analysis iterations (see Figure 4).

Source: Own elaboration

8. Safety and sustainability assessment

Safety and sustainability assessments are the methods for characterisation of the systemic environmental and toxicological impacts of processes, products, and their associated chemical releases. Recognising the fundamental differences between safety and sustainability but also the strengths that make each approach unique is important in the context of SSbD. The two approaches should be understood as complementary to each other and should be developed separately to produce a robust, reliable and adequate SSbD assessment. The safety and sustainability assessment part consists of:

- **Intrinsic physical and (physico-)chemical properties** (Chapter 9): As common ground for safety and sustainability assessment, it covers the collection of physical and chemical characteristics of chemicals and materials. These properties determine how chemicals and materials behave under different conditions and how they interact with other chemicals and materials. These properties are influenced by the molecular structure, substance composition, physical dimensions and other properties.

- **Safety assessment** (Chapter 10): Safety assessment quantifies both the potential of exposure and hazard associated with a specific chemical or material in specific scenarios to generate an absolute estimate of risk and reports results relative to maximum threshold levels, where these are available. The chapter focuses on chemical safety covering the analysis of the intrinsic properties of the chemical/material to understand its hazard profile in combination with the exposure (human health and environment), aspects throughout the life cycle, including the production, manufacturing processes, other downstream processes (including End of Life) and final application and use of the product which the chemical/material is part of. Process related safety is an example of the holistic safety from a specific life cycle stage. SSbD includes all process-related safety considerations identified in the innovation scenario, from e.g. chemical risks associated with the (re)designed chemical or material as well as its precursors and other chemicals employed, to safety considerations of the technologies behind the processes.

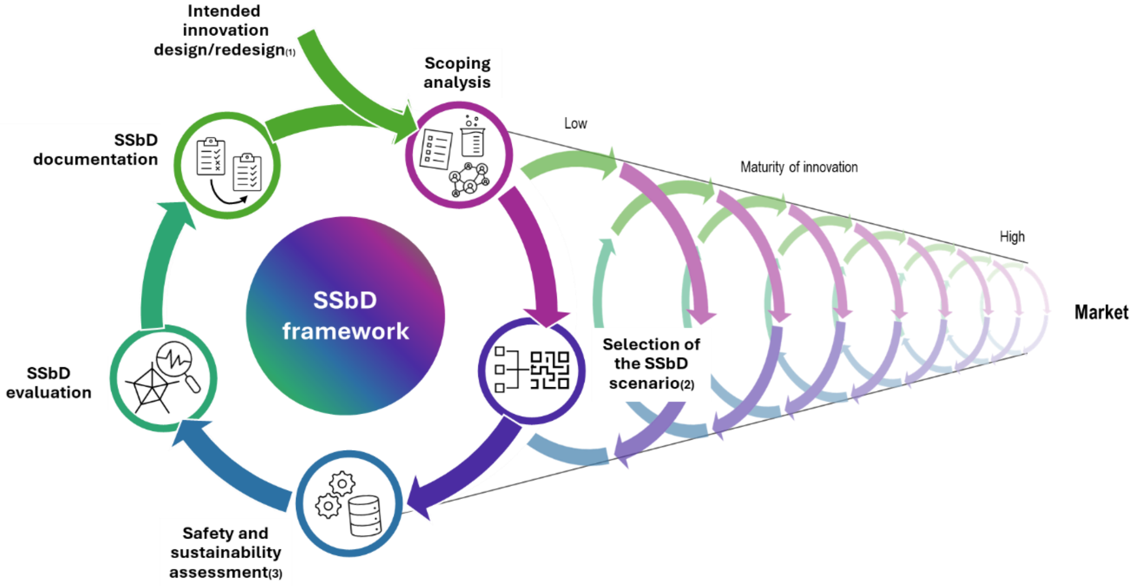
- **Sustainability assessment** focused on the overall processes related to the chemical/material and its life cycle:

    - **Environmental sustainability assessment** (Chapter 11): it evaluates the environmental impacts along the entire chemical/material life cycle by means of Life Cycle Assessment (LCA), assessing several impact categories such as climate change and resource use, for, among others, the production, the downstream processes and final application and use of the chemical/material. Process-related sustainability, provides an example of how environmental hotspots could be identifiable in early stage of the technological and process innovation; moving toward higher stage, the identification of environmental pressures and impacts associated with the industrial plants will be also possible.

- **Socio-economic sustainability assessment** (Chapter 11.3): it describes how to assess aspects related to social fairness (e.g. working conditions and human rights) and competitiveness (e.g. vulnerabilities in the supply chain, skills shortages and Life Cycle Costs). The assessment includes both social risk assessment, the identification of Critical Raw Materials and the assessment of societal costs during the life cycle of a chemical or a material.

The safety and sustainability assessments can be tailored based on the identified scenario (Chapter 7). Safety and sustainability assessment can be performed in parallel, in an iterative and tiered manner, as information becomes available along the life cycle of the chemical/material and depending on the specificity of the assessment (as illustrated in the Figure 10 below).

Figure 10. Iterative and tiered approach of the SSbD framework.



(1) Innovations can be triggered for example by the need of improving existing portfolios, new market/consumer requests, new ambitions and priorities and/or policy priorities
(2) Key moment where the tailored safety and sustainability assessment is defined according to the outcomes of the scoping analysis
(3) The safety and sustainability assessment are tailored based on the *selected SSbD scenario*

Source: Own elaboration

A set of general scenarios for the safety and sustainability assessment is shown in Figure 11. These scenarios are tailored according to the maturity of the innovation[4], and the related availability of information/data, reflecting the iterative and tiered nature of the SSbD framework.

Since the SSbD scenario identified is case specific, the practitioner will need to complement this representation of the tiered approach according to the specificity of the identified scenario. Indeed, further adjustments will depend on the other elements identified through the scoping analysis such

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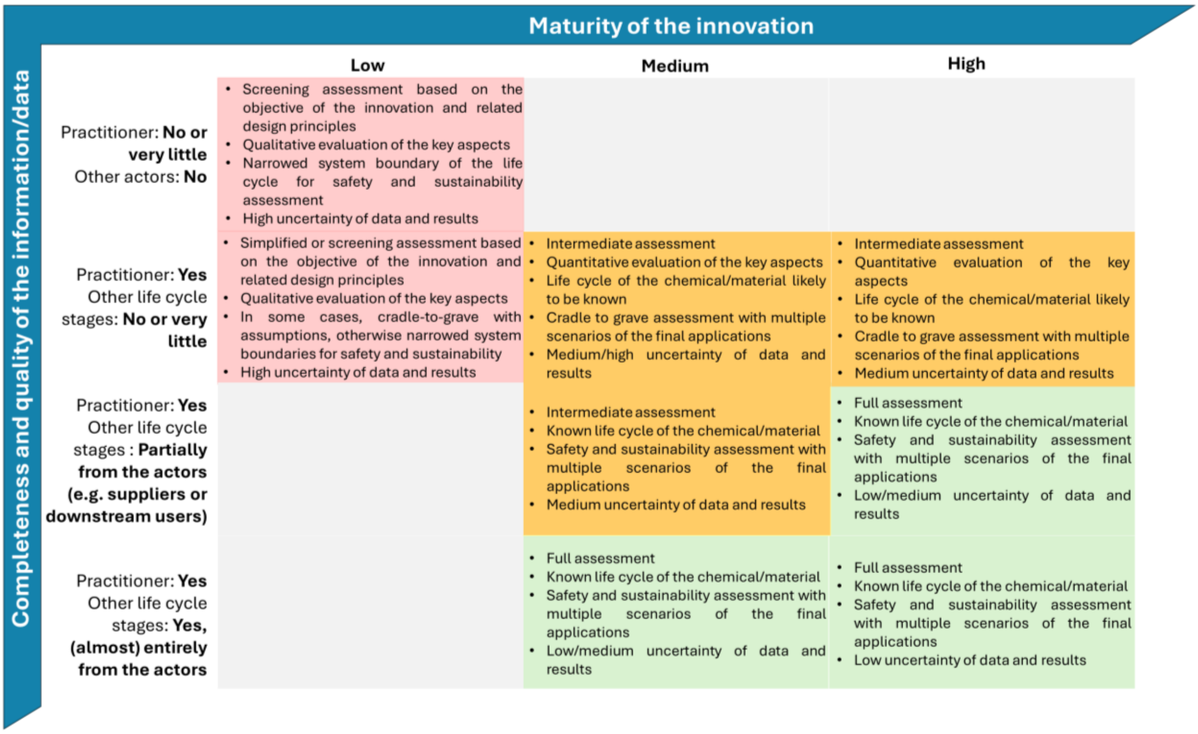
[4] The maturity of the innovation will be defined and evaluated by the assessor or innovator according to different used approach, such as Cooper stage-gate, Technological Readiness Level (TRL), or regulatory readiness level

as the innovator and its position along the life cycle, key goal of the (re)design, the sector where the SSbD framework is implemented.

Further information about the tiered assessment for safety and sustainability aspects are provided in chapters 10 and 11.

Figure 11. Tiered approach of the SSbD assessment based on the maturity of the innovation and the availability of the data.



Maturity of the innovation

Completeness and quality of the information/data

	Low	Medium	High
Practitioner: **No or very little** Other actors: **No**	• Screening assessment based on the objective of the innovation and related design principles • Qualitative evaluation of the key aspects • Narrowed system boundary of the life cycle for safety and sustainability assessment • High uncertainty of data and results		
Practitioner: **Yes** Other life cycle stages: **No or very little**	• Simplified or screening assessment based on the objective of the innovation and related design principles • Qualitative evaluation of the key aspects • In some cases, cradle-to-grave with assumptions, otherwise narrowed system boundaries for safety and sustainability • High uncertainty of data and results	• Intermediate assessment • Quantitative evaluation of the key aspects • Life cycle of the chemical/material likely to be known • Cradle to grave assessment with multiple scenarios of the final applications • Medium/high uncertainty of data and results	• Intermediate assessment • Quantitative evaluation of the key aspects • Life cycle of the chemical/material likely to be known • Cradle to grave assessment with multiple scenarios of the final applications • Medium uncertainty of data and results
Practitioner: **Yes** Other life cycle stages : **Partially from the actors (e.g. suppliers or downstream users)**		• Intermediate assessment • Known life cycle of the chemical/material • Safety and sustainability assessment with multiple scenarios of the final applications • Medium uncertainty of data and results	• Full assessment • Known life cycle of the chemical/material • Safety and sustainability assessment with multiple scenarios of the final applications • Low/medium uncertainty of data and results
Practitioner: **Yes** Other life cycle stages: **Yes, (almost) entirely from the actors**		• Full assessment • Known life cycle of the chemical/material • Safety and sustainability assessment with multiple scenarios of the final applications • Low/medium uncertainty of data and results	• Full assessment • Known life cycle of the chemical/material • Safety and sustainability assessment with multiple scenarios of the final applications • Low uncertainty of data and results

Source: Own elaboration

9. Intrinsic physico-chemical properties

An important element that forms the basis for both the safety and sustainability assessment is the physico-chemical characterisation of the chemical/material under assessment.

Physico-chemical properties describe the combination of physical and chemical characteristics of a chemical or material. These properties are influenced by the molecular structure, substance composition, physical dimensions and other properties.

They determine the reactivity of the chemical/material, how it behaves under different conditions and how it interacts with other chemicals and materials, as well as its 'transformation products' (Box 3) and its performance with regard to safety and sustainability aspects.

Hence, a good characterisation of the intrinsic physico-chemical properties of the chemicals/materials in the SSbD system is of paramount importance for finding innovative solutions that provide a desired function while ensuring their safety and sustainability throughout their entire life cycle.

Box 3. Consideration of 'transformation products' in the chemical/material characterisation.

A 'transformation product' (TP) is an element, ion or molecule formed from a particular chemical or material as a result of metabolism, chemical reactions or environmental processes[5].

The consideration of TPs in the safety and sustainability assessment is critical to ensure a comprehensive environmental and human health protection, as some TPs exhibit higher (eco)toxicological risk than the parent chemical/material (Scheringer, 2011), and vice versa.

Within the SSbD framework, early identification of possible TPs might be useful, for example to re-orient the innovation. In any case, when considering the uncertainty related to the safety assessment, TPs should be considered.

Examples of physico-chemical properties of chemicals that affect e.g. their safety, can be found in current legislation, but properties not yet explicitly addressed in a regulatory context may also be relevant for the SSbD practitioner.

In the context of safety, physico-chemical data are used to assess the physical hazards (e.g. flammability) and help predict possible toxicological or environmental hazards.

They also help to predict fate and behaviour relevant in the determination of exposure to humans and the environment in the different stages of the chemical/material lifecycle (Example in Box 4).

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[5] Based on EFSA definition (https://www.efsa.europa.eu/en/glossary/transformation-product)

Box 4. Example of how information on physico-chemical data may help to understand the fate and behaviour of a chemical.

A chemical's octanol–water partition coefficient (K_{ow}) represents a measure of its hydrophilicity/lipophilicity. It can help to predict:

- outcomes of other physico-chemical tests: K_{ow} is generally inversely related to water solubility. In general, K_{ow} tends to increase with the molecular weight of a substance. Generally, substances with a high log K_{ow} will be hydrophobic and have low water solubilities. Substances with negative log K_{ow} will be hydrophilic and have high water solubilities.
- the toxicokinetic behaviour: K_{ow} indicates the potential for absorption across biological membranes and for passive diffusion (e. g. useful for prediction of dermal absorption). It provides information on the potential for accumulation in the body.
- environmental behaviour: K_{ow} is a very important parameter for predicting the distribution of a substance in environmental compartments (water, soil, sediment, air, biota, etc.). Substances with high K_{ow} values tend to adsorb more readily to organic matter in soils or sediments because of their low affinity for water.

The octanol–water partition coefficient (K_{ow}) is not well-suited for nanomaterials, as their behaviour is driven by particle properties like size and surface characteristics rather than partitioning at molecular level. Measuring K_{ow} for nanomaterials is also problematic due to issues like agglomeration, sedimentation, and poor reproducibility, making it an unreliable indicator of their environmental fate or bioaccumulation potential.

10. Safety assessment

Safety assessment is the process by which the potential risks posed by chemicals and materials to human health and the environment throughout their life cycle are systematically evaluated. The process seeks to ensure that chemical and materials can be developed, used, and managed at end of life in a safely manner.

From a **holistic perspective**, safety assessment can be approached from multiple angles, depending on its goal and scope (Figure 12). It may focus on the inherent properties of the chemical or material itself (see section 10.2), or on specific life cycle stages, such as process safety during manufacture (see section 10.4), formulation safety, or product safety during use. It can also be framed from the perspective of different exposed populations or environmental receptors, including occupational safety for workers, consumer safety for product users, and environmental safety for ecosystems.

Together, these perspectives provide a comprehensive understanding of potential hazards, exposure routes, and risks, enabling informed decision-making to ensure safe design, handling, and disposal of chemicals and materials.

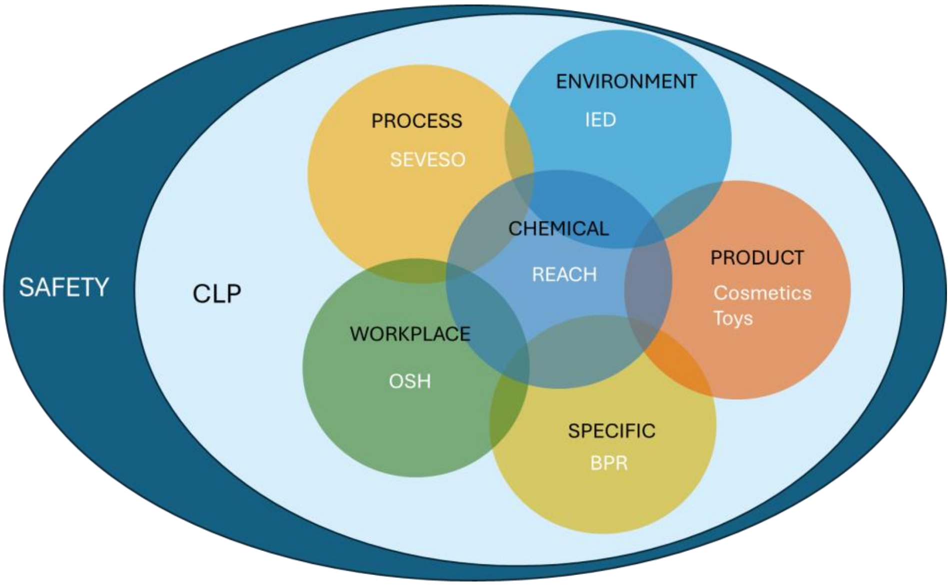
Figure 12. Safety components and perspectives in SSbD.

Source: Own elaboration

Numerous legal and regulatory frameworks have been established at national and international levels to address these safety aspects. These frameworks aim to protect human health and the environment, promote safer products, and ensure transparency and accountability in chemical development, processing and use. In Europe it encompasses various legal frameworks with a focus on identifying, evaluating, and minimizing potential risks to humans and the environment and addressing different sectors and duty holders. Annex 4 gives examples of the most relevant legislations established in the EU to assess chemical safety, workplace safety, environmental safety, process safety and product safety.

The Figure 13 below, illustrates in a simplified manner the European safety framework related to chemicals. In the European Union, REACH and CLP can be considered as the overarching chemical and material safety regulations. Other legislative frameworks are based on elements of REACH and CLP to further develop specific process and product safety requirements like for example SEVESO and IED (Industrial Emission Directive) addressing major chemical accidents and environmental aspects in processes, OSH (Occupational Safety and Health) addressing workers safety in workplaces, Toys and Cosmetic Products Regulations addressing consumer safety in products and other regulations addressing specific products like BPR (Biocidal Product Regulation) or medical devices.

Figure 13. Simplified illustration of the safety framework related to chemicals with examples of relevant legislation.



Source: Own elaboration

The individual pieces of legislation vary in their objectives and scope, which means that also e.g. data requirements, chemical/material life cycle stages and target populations or ecosystems vary. Despite these differences, all are underpinned by a common scientific methodology and the elements to perform a safety assessment are in all cases the same (Hazard identification, likelihood and severity of the exposure, assessment and management of the risk). Understanding this common base is essential for ensuring consistency and fostering innovation in chemical and materials safety across diverse domains.

However, the SSbD practitioner should be aware of these differences as the innovation progresses, and the market scenarios become clearer. In addition, the practitioner should consider the added value of the innovation within a holistic perspective, going beyond individual hazards, chemicals or sustainability performance. Box 5 provides an example of how a holistic perspective supports the implementation of the SSbD framework.

Box 5. Example of how a holistic perspective supports the implementation of the SSbD framework.

Biocidal products are often perceived as problematic from a safety and sustainability perspective, primarily because their active substances are often inherently hazardous, (designed to kill or control harmful organisms for example insects, micro-organisms or rodents), and risk management relies on controlling the exposure (e.g. the amount). Similarly, if considered in isolation from the active substance's life cycle perspective, without context to their broader societal benefits, some biocidal products may appear to have a high environmental burden due to their formulation, use, and end of life impacts.

Biocidal products provide significant and indispensable benefits. These products contribute directly to public health, hygiene, food safety, and infrastructure protection, and by doing so, support the achievement of multiple UN Sustainable Development Goals (SDGs) (UN, 2015) . For example:

Disinfectants used in hospitals and public settings play a vital role in preventing infections (SDG 3), reducing the spread of diseases like COVID-19, and other healthcare-associated infections.

Preservatives extend the life of materials such as paints, construction products, and wood, reducing the need for frequent replacement and thereby supporting sustainable consumption and production (SDG 12).

Biocidal treatments in water systems, like legionella control in cooling towers, are essential for maintaining safe and clean water (SDG 6).

The holistic and integrated implementation of the SSbD framework allows the development of products like biocides by optimising their efficacy, while minimising exposure, and managing life cycle impacts. While biocidal products must be carefully assessed and controlled due to the inherent hazards of most of their active substances, they should also be evaluated considering their societal and environmental value.

10.1. Aspects, and indicators definition

Despite differences in the legal and procedural context, chemical safety assessments across sectors follow a shared, four-element process:

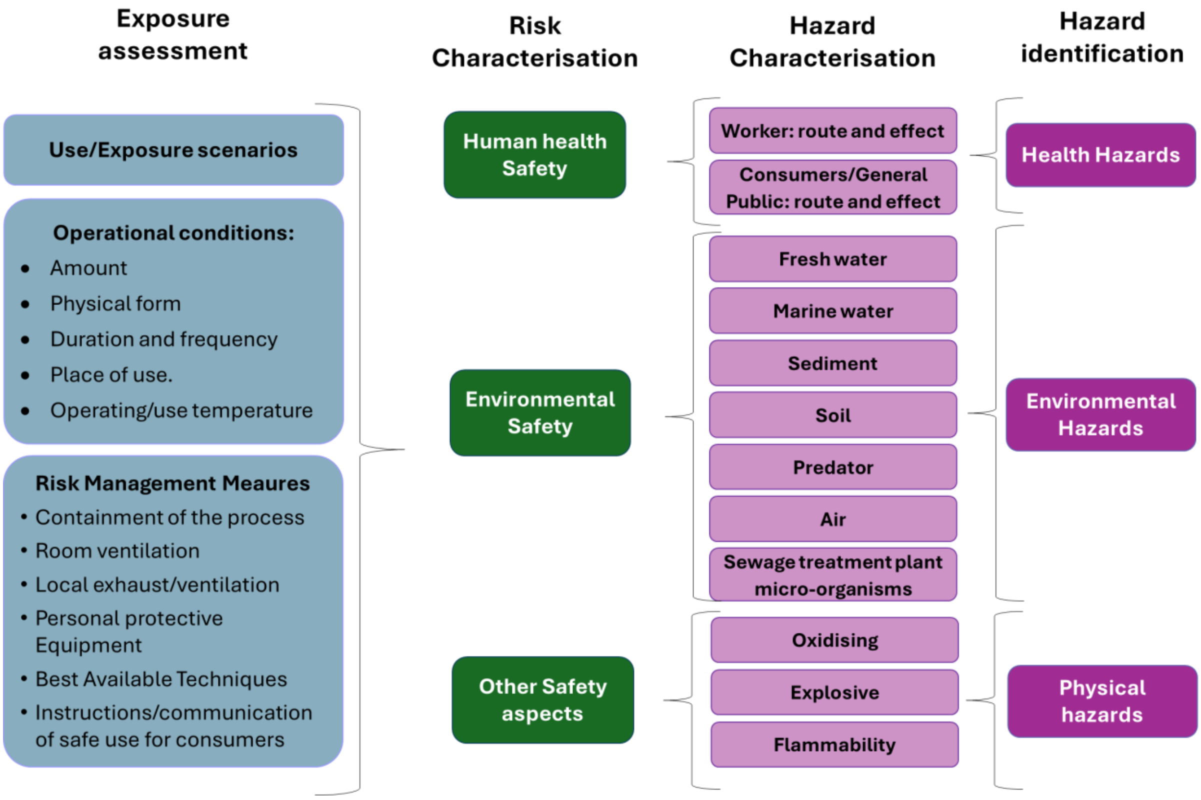
- **Hazard Identification:** Determination of whether the intrinsic properties of a chemical may cause harm (e.g. carcinogenicity, reproductive toxicity, ecotoxicity).
- **Hazard Characterisation (or Dose–Response Assessment):** Establishes the relationship between the dose or concentration of a chemical and the severity or probability of adverse effects. This includes identifying critical effects and determining reference tolerable exposure limit.
- **Exposure Assessment:** Estimates the magnitude, frequency, duration, and route of exposure to the chemical for humans or environment for the relevant exposure pattern (population, route, and duration of exposure) and each relevant health effect (local and systemic effects) under realistic or worst-case scenarios.

  In order to ensure safety, actions or controls to reduce the likelihood or severity of harmful effects arising from the hazard and exposure can be implemented (**Risk Management Measures)**

- **Risk Characterisation:** Integrates hazard and exposure information to estimate the likelihood and severity of harm under specific use conditions. Safety can be expressed based on Risk Characterisation Ratios (RCRs) which compare the estimated exposure to a chemical with the tolerable exposure limit, where the latter are available.

Each of the four elements relies on various aspects. Their characterisation requires integrating diverse data streams from multiple sources (Figure 14).

Figure 14. Aspects to be considered for the hazard identification and characterisation, exposure assessment and risk characterisation.



Source: Own elaboration

In a Full SSbD approach, these aspects must, in principle, be considered at each stage life cycle stage of the SSbD system (see Box 1), taking into account the different chemicals and materials involved together with their intrinsic properties, and the diverse exposure scenarios and the contributing activities that may lead to potential exposure.

Since there is no “one-size-fits-all" approach for safety assessment, the assessor must make several methodological choices at each step of the innovation process. These choices can lead to potentially different conclusions, thus guiding innovation through different pathways. Therefore, for transparency and traceability purposes documenting the different decisions taken during the innovation process is paramount.

The problem formulation (Box 6) improves transparency and traceability by laying out assumptions, limitations, and reasoning in each iteration of the assessment.

Box 6. The importance of Problem formulation for safety assessment to improve efficiency and transparency.

Problem formulation is the essential step in any safety assessment. It defines the purpose, scope, and strategy of the assessment. It defines what is being assessed, why, and how, ensuring that the assessment is focused and efficient. Without clear problem formulation, safety assessments risk becoming too broad, unfocused, or misaligned with the goals.

In each iteration of the innovation the problem formulation:

- Clarifies the Purpose: Specifies whether the assessment is intended to support overall safety or to address a specific aspect or indicator resulting from the (re)design action. It also defines the focus of the assessment—such as a particular chemical or material, life cycle stage, exposed population, or environmental receptor—as well as the type of assessment to be conducted (qualitative, semi-quantitative, or quantitative) and the associated uncertainty considerations.
- Frames the scope (the system) by specifying what chemicals, materials, processes and products are addressed, as well as the scenarios, populations, and effects that are relevant.
- Identifies goals: What aspects need to be assessed and/or improved.
- Defines criteria to align with the goal and the purpose: weighting, decision rules etc.
- Selects and focuses the assessment on relevant hazard endpoints or exposure routes, population exposed in the use (processes, products….), etc.
- Helps to identify which data to collect or generate, avoiding unnecessary testing and focusing on priority uncertainties.
- Determines the approach (deterministic or probabilistic), data sources, models, and assumptions to be used.

A robust problem formulation allows for a tiered approach starting with existing data, or conservative models for initial screening, and refining with new data and use of higher-tier models when needed.

Importantly, problem formulation also frames uncertainty and variability, helping assessors decide when expert judgment, sensitivity analysis, or probabilistic modelling should be employed.

The problem formulation in innovation must be understood as an iterative process that takes place as data and information become available and refinement is possible. These iterations support a tiered safety assessment in innovations.

The tiers represent the progression in the confidence of the assessment, determined by the availability and quality of data, the robustness of the methods used, the strength of supporting evidence, the time investment required, and the expertise necessary for data collection and interpretation.

10.2. Safety assessment in innovation

Therefore, the decision of the best approach to be taken for the safety assessment will depend on the entry point of the innovation into the assessment process. This will be defined in each iteration with the different elements of the scoping analysis. Among these elements, the system definition, the type of innovation (incremental vs breakthrough) and the applied (re)design (molecular, process or product) has a special importance for the safety assessment (Box 7).

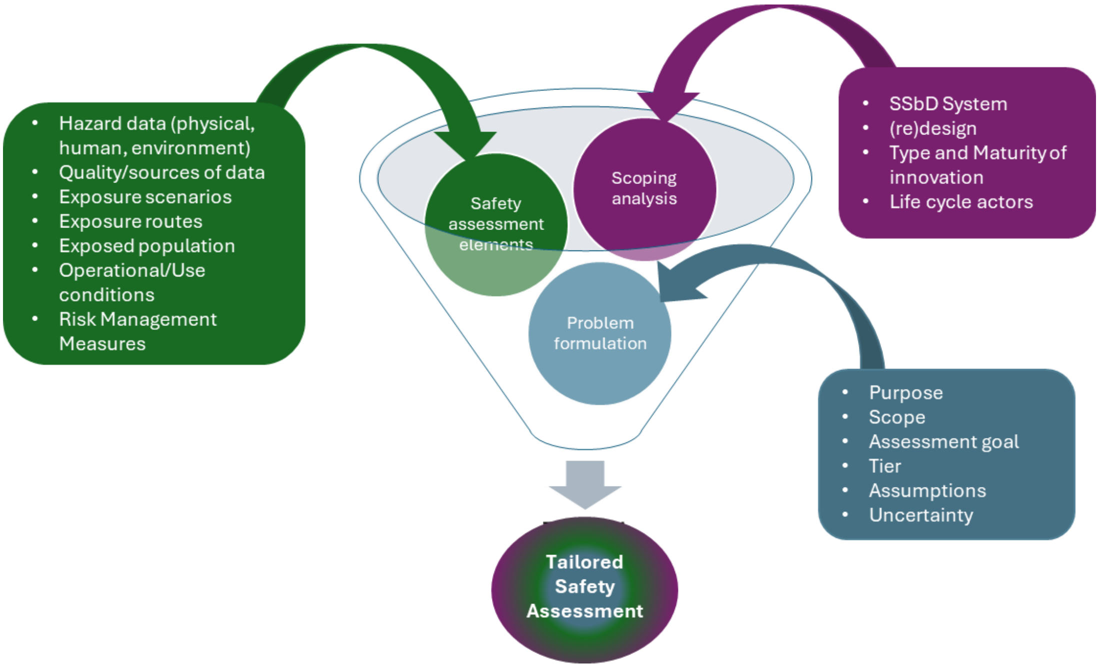
Box 7. The importance of a robust characterisation of the chemical/material for the safety assessment.

Chemical and material characterisation is the cornerstone of safety assessment. It ensures that what is being assessed is well understood, enables accurate modelling and testing, and supports transparent, science-based decision-making throughout the risk assessment process.

Single, pure chemicals and materials do not exist in the real world, instead substances can be mono or multi-constituent chemicals, UVCB substances (substances of unknown or variable composition, complex reaction products or of biological material) and materials can be multicomponent materials or Advanced Materials. Without a robust characterisation, any subsequent hazard, exposure, or risk assessment may be unreliable or misleading (ECHA, 2023). Safety assessment of UVCB substances (substances of unknown or variable composition, complex reaction products or of biological material) or **Advanced Materials**, such as nanocomposites, hybrid materials, and functionalised surfaces, requires a tailored and often more complex approach than assessment of chemicals that have only one molecular structure. Chemicals such as UVCB substances and Advanced Materials are often composed of multiple components with distinct properties, functions, and interactions, which may not be predictable from the characteristics of the individual components alone. Therefore, the approach for the assessment is usually to start with a comprehensive material characterisation. A detailed understanding of the material's composition, structure, physico-chemical properties and transformations under realistic conditions is fundamental for the assessment. The characterisation must consider not only the pristine material, but also its form in relevant media and after environmental or biological interactions.

The problem formulation complements the scoping analysis by adding granularity and considering additional information. Figure 15 illustrates how the safety assessment is tailored based on the scoping analysis and problem formulation elements.

Figure 15. Path tailoring based on the scoping analysis elements and complemented with the problem formulation mentioned in Box 6.



- Hazard data (physical, human, environment)
- Quality/sources of data
- Exposure scenarios
- Exposure routes
- Exposed population
- Operational/Use conditions
- Risk Management Measures

- SSbD System
- (re)design
- Type and Maturity of innovation
- Life cycle actors

- Purpose
- Scope
- Assessment goal
- Tier
- Assumptions
- Uncertainty

Source: Own elaboration

Two main approaches can be considered depending on the different elements and available data and information at the beginning of the innovation, hazard-based (also called generic) risk approach and exposure-based risk approach. Regardless of the initial approach, a comprehensive and robust safety assessment should be pursued as the innovation progresses and data and information are generated.

In the hazard-based risk approach, the nature of the hazard will determine the possible use(s) of a chemical/material. Thus, the hazard is identified and characterised first. A hazard-based approach can be a straightforward starting point for safety assessment, especially when the innovation refers to substances and mixtures already on the market, thus already classified. Regulation 1272/2008 on Classification, Labelling and Packaging of substances and mixtures (CLP Regulation) (EC, 2008a) builds on criteria based on (eco)toxicological gathered and generated during the hazard identification (see Hazard identification) data and assigns hazard classes and categories accordingly.

SSbD hazard-based criteria (Table 5) are also based on these CLP hazard classes and categories. The purpose of the hazard-based SSbD criteria is to raise early awareness on certain aspects that the innovator/SSbD practitioner should consider when innovating to prevent or anticipate future consequences and requirements in alignment with EU policy objectives.

Table 5. Hazard-based SSbD criteria and considerations in alignment with the EU policy objectives.

Hazard-based SSbD Criteria	**Related Considerations -** relevant for decision making on the role of the chemical or material in the innovation, and for the scoping analysis in the initial and subsequent iterations of the SSbD cycle
Criterion H1 that includes the most harmful substances (according to CSS (EC, 2020a), including substances meeting hazard criteria that can be used to identify substances of very high concern (SVHC) according to REACH Art. 57(a-f) (EC, 2006).	Innovators should consider impacts of the identified properties and be aware that chemicals and materials which do not pass the Criterion H1 are subject, or could become subject, to legislation that: ▪ Bans, restricts or at least discourage their use, except for derogated uses, e.g, those considered essential for society ▪ Imposes conditions on safely use and requires emissions/exposure to be controlled along the whole life cycle ▪ Requires that activities are undertaken to identify or develop alternatives as soon as possible, so they can be substituted and their use phased out as soon as alternatives are available that are less hazardous, more sustainable and economically and technically viable. ▪ Implies their use and presence has to be tracked through their life cycle. ▪ Requires them to be (re-)designed to reduce their adverse effects
Criterion H2 that includes substances of concern, as described in CSS (EC, 2020a), defined in the Article 2(27) of ESPR (EC, 2024a) and that are not already included in Criterion H1.	Innovators should consider impacts of the identified properties and be aware that the chemicals and materials that do not pass Criterion H2 are subject, or could become subject, to legislation that: Imposes conditions on safe use and requires emissions/exposure to be controlled along the whole life cycle: ▪ Requires that they are substituted as soon as alternatives are available that are less hazardous, more sustainable and economically and technically viable ▪ Implies their use and presence has to be tracked through their life cycle ▪ Requires them to be (re-)designed to reduce their adverse effects
Criterion H3 that includes the other hazard classes not part already in Criteria H1 and H2.	Innovators should consider impacts of the identified properties and for the chemicals and materials that do not pass Criterion H3 consider: ▪ To flag them for internal review to find methods to use them in ways that reduce their toxic effects ▪ How to ensure their safe use along the life cycle until alternatives are available that are less hazardous, more sustainable and economically and technically viable.

Source: Own elaboration

Hazard-based criteria can be used for screening and flagging hazard related issues, especially in process and product related innovations in which the (re)design actions are focused on either reducing the exposure or using already on the market chemical alternatives.

However, this approach is not applicable to chemicals and materials for which classification information might not yet be available and other approaches to the safety assessment might be considered more appropriate (e.g. tiered hazard identification approach or exposure identification approach). Moreover, hazard classification does not provide specific data needed to support the hazard characterisation for a robust safety assessment which, together with the sustainability assessment, provides the holistic SSbD assessment (Box 5).

Exposure assessment

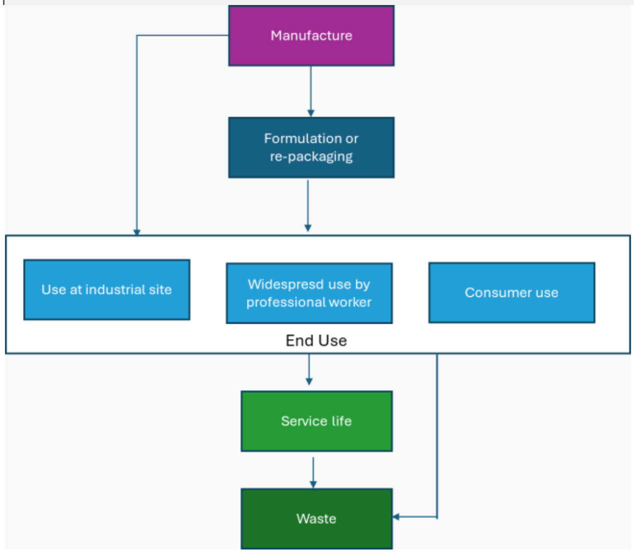
In safety assessment, the exposure determines the risk as much as the hazard. In the exposure-based risk approach, exposure is known, and hazards can be assessed in a targeted way based on this exposure.

To understand and estimate the exposure it is important to specify the use. Any activity for which there is a potential for human or environmental exposure to a chemical/material is defined under REACH (European Parliament and the Council, 2006), as “use”. Use means any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, production of an article or any other utilisation. Although not regarded as uses under REACH, the life stages of manufacturing and waste must be considered in the SSbD chemical safety assessment as well.

The exposure assessment therefore starts with the **identification of the use case** and the development of the **exposure scenarios** that raise a concern about the safety to the human health and / or the environment (including human health through the environment). The development of the exposure scenarios starts by describing the use in the different life cycle stages to the extent that is possible. Methods such as the use descriptors developed in the context of REACH can support the SSbD practitioner in defining the exposure scenarios relevant for the processes in which the chemicals and materials are used and the products and applications in which they are part of, in a harmonised manner. These descriptors define the life cycle stage (LCS) in which the use takes place (Box 8), the process conditions (PROC), the product category (PC), the sector of use (SU), environmental release category (ERC) in which the use take place, the article category, and the technical function (TF).

Box 8. Example of a Life cycle of a substance described in guidance for the EU REACH Regulation.

According to REACH guidance R12 there are four basic steps or stages in the **life cycle of a substance** (LCS) to which a use can be assigned: manufacture, formulation or re-packing, end-use (article) service life and waste as illustrated below.



The life cycle starts with the activities of the first actor in the life of a substance, the manufacturer. It continues with the description of the activities of formulators, where relevant. Then activities undertaken by different end-users of the substance as such or in a mixture i.e. industrial workers, professional workers or consumers are to be described. The last stage of the life cycle of the substance to be considered for use description purposes is the end-use or the service life.

End of life of the substance is when is consumed in a process by reaction during use (including intermediate use), is emitted to waste streams or the environment or is included into an article.

Source: Own elaboration

The waste stage (disposal or recovery operations,) as it is not considered a "use" in REACH, is not covered by the guidance R.12 guidance but for the purpose of safety assessment and in the context of the SSbD should be regarded as a downstream process or activity.

The safety requirements for recovered and recycled chemicals and materials (secondary chemical/materials) are the same as the those for primary chemicals and materials.

Not all descriptors are always needed like for example for intermediates, where the life cycle is often short and confined to closed systems within industrial settings (Box 9).

Box 9. Intermediates as short life cycle substances.

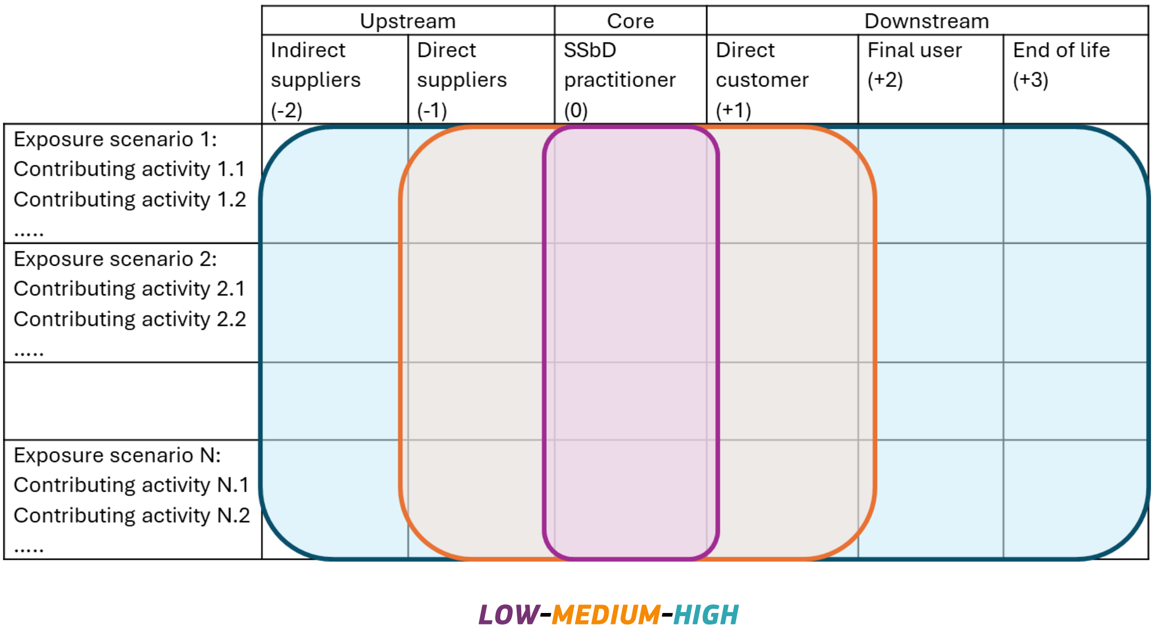
Intermediates are substances that are manufactured for and used solely for chemical processing to be transformed into another substance (according to Art 3(15) of REACH). In the context of the SSbD system, intermediates can be considered also as precursors.

The safety assessment of intermediate substances follows the same methodology that is applied to final chemical products. However, the life cycle of intermediates is often short and confined to closed systems within industrial settings. They should never have any service life described, as by definition they are transformed during industrial use into another substance. Therefore, they typically do not enter consumer or environmental pathways.

The risk assessment for intermediates focuses on the specific conditions of manufacture and use, with particular attention to whether the substance is handled under strictly controlled conditions (SCCs).

In the context of applying the SSbD Framework, at the early stages of innovation, one or more pieces of information regarding the use of the chemical/material under assessment are often missing. Table 6 illustrates how Information on use and exposure evolves along the life cycle, becoming more detailed as exposure scenarios are developed and refined. As innovation progresses and engagement with actors across the life cycle increases, both upstream and downstream information becomes more complete and more reliable. Starting with the exposure scenarios of single actor/innovator and core SSbD practitioner and the exposure scenarios are expanded upstream and downstream in the value chain as innovation progresses to align with the SSbD framework principles.

Table 6. Level of application of considering the life cycle of a chemical/material.



	Upstream		Core	Downstream		
	Indirect suppliers (-2)	Direct suppliers (-1)	SSbD practitioner (0)	Direct customer (+1)	Final user (+2)	End of life (+3)
Exposure scenario 1: Contributing activity 1.1 Contributing activity 1.2						
Exposure scenario 2: Contributing activity 2.1 Contributing activity 2.2						
Exposure scenario N: Contributing activity N.1 Contributing activity N.2						

Source: Own elaboration

Besides describing the use, the physico-chemical properties (see chapter 9), the operational conditions in which these uses take place and the Risk Management/Mitigation Measures (RMM) need to be considered for the **exposure scenario and estimation**.

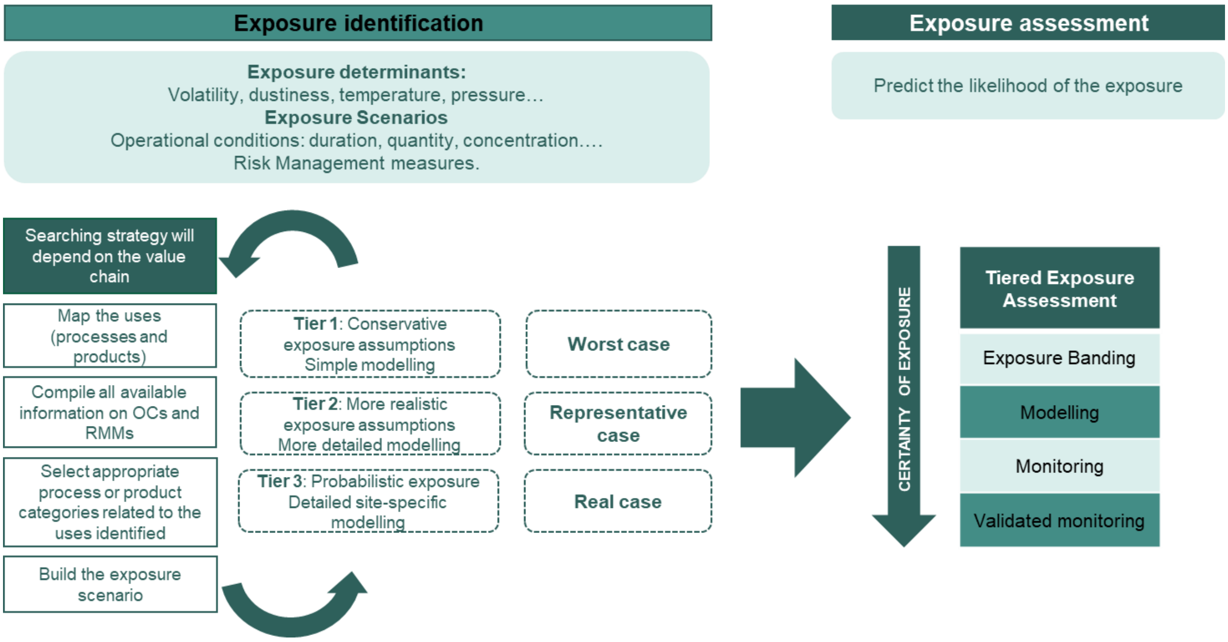
Operational conditions and the risk management measures (Table 7) will determine the risk of exposure of workers, consumers, and the environment.

Table 7. Generic Operational Conditions and Risk Management measures

Operational conditions	**Risk Management/Mitigation Measures**
Amount (i.e. percentage (w/w)) of chemical/material in the process or product Physical form Duration and frequency of the exposure (processing or use) Place of use. The environment in which the exposure takes place Operating/use temperature	Containment of the process/Use Room ventilation Local exhaust ventilation Personal protective Equipment: Respiratory protection, dermal protection, face and eye protection Best Available Techniques Instructions/communication of safe use for consumers

The exposure assessment can be performed in a tiered approach as information to build the exposure scenarios becomes more realistic (Figure 16). In Tier 1, exposure is assessed using worst-case assumptions o quickly identify red flags. This tier is intentionally conservative and requires minimal input data (e.g. default values, generic use scenarios). If no risk is identified, the assessment may stop here. If potential concerns are flagged, the assessment moves to Tier 2, where more realistic use conditions and risk management measures, refined models, and measured or scenario-specific data are incorporated (real concentrations, frequency of use, or site-specific release factors). Tier 3 involves the highest level of refinement, often using quantitative monitoring data, advanced exposure modelling, and occupational/environmental measurements.

Figure 16. Exposure assessment tiered approach.



Source: Own elaboration

Hazard assessment

Hazard assessment is the combination of the hazard identification that determines whether a chemical can cause harm based on its inherent properties, and hazard characterisation that describes the nature and severity of the adverse effects and defines the dose–response relationship. For processes hazard assessment also includes e.g. identification of failure of processing equipment.

Hazard identification

The hazard identification follows a tiered approach starting with screening approaches in Tier 1. If the chemical/material is already on the market existing data sources can be used, such as Safety Data Sheets (SDS), regulatory classification, public databases, and QSAR models or read across from structurally similar substances. The focus is on quickly flagging substances with known or suspected hazardous properties. When working with existing substances, much of this information may already be available in databases, e.g. hosted by ECHA. For new or modified materials, particularly at early innovation stages, data may be sparse, and hazard identification relies on conservative assumptions and predictive tools to identify potential areas of concern.

As the innovation progresses and more information becomes available, the process moves into higher tiers, involving more refined and targeted testing strategies. Tier 2 may include in vitro methods or validated new approach methodologies (NAMs) for specific endpoints, while Tier 3 may involve more comprehensive in vivo studies or integrated approaches to testing and assessment (IATAs) where justified and ethically permissible (Figure 17).

Hazard characterisation

A toxicological dose-response descriptor is the term used to identify the relationship between a specific effect of a chemical substance and the dose at which it takes place. Dose-response descriptors are usually expressed as Lethal Concentration 50% (LC50), Lethal Dose 50% (LD50), No Observed Adverse Effect Level (NOAEL), No Observed Adverse Effect Concentration (NOAEC) etc.

Hazard characterisation builds on the (eco)toxicological test data and dose-response descriptors to define specific criteria for safety assessment and setting this way the absolute boundaries for humans and environment, based on the scientific state of the art. The dose-response descriptors are used for deriving the no-effect threshold levels for human health (i.e. DNEL) and the Predicted No Effect Concentration (PNEC) for the environment. These are the levels above which a particular human population (e.g. workers, consumers) and the environmental compartments (soil, sediment, water, air, etc.) should not be exposed. DNELs are derived for each relevant exposure pattern (population, route, and duration of exposure) and each relevant health effect (local and systemic effects). They will vary for each population, since some (e.g. children, pregnant women) require more protection than others, for each different route of exposure (oral, dermal, inhalation), and possibly also depend on the level, duration and frequency of the exposure. Table 8 gives an overview of exposure patterns for humans and the environment.

Table 8. Overview of exposure patterns for human population and environment.

Human health		
Population	**Duration**	**Effect**
Workers	Acute	dermal, local effects
		inhalation, local effects
		inhalation, systemic effects
	Long term	dermal, systemic effects
		inhalation, systemic effects
		dermal, local effects
		inhalation, local effects
Consumers/General Public	Acute	dermal, local effects
		inhalation, local effects
		inhalation, systemic effects
	Long term	dermal, systemic effects
		inhalation, systemic effects
		oral, systemic effects
		dermal, local effects
		inhalation, local effects
Environment Compartment		
Aquatic compartment		Fresh Water
		Marine Water
Sediment		Fresh water sediment
		Marine sediment
Terrestrial (Soil) compartment		
Sewage treatment plant micro-organisms		
Air compartment		Biotic
		Abiotic
Predator		Fish eating predators
		Worm eating predators
Man via environment		Inhalation Ingestion

Source: ECHA R.8 2012), R.10 (2008) and R16 (2016)

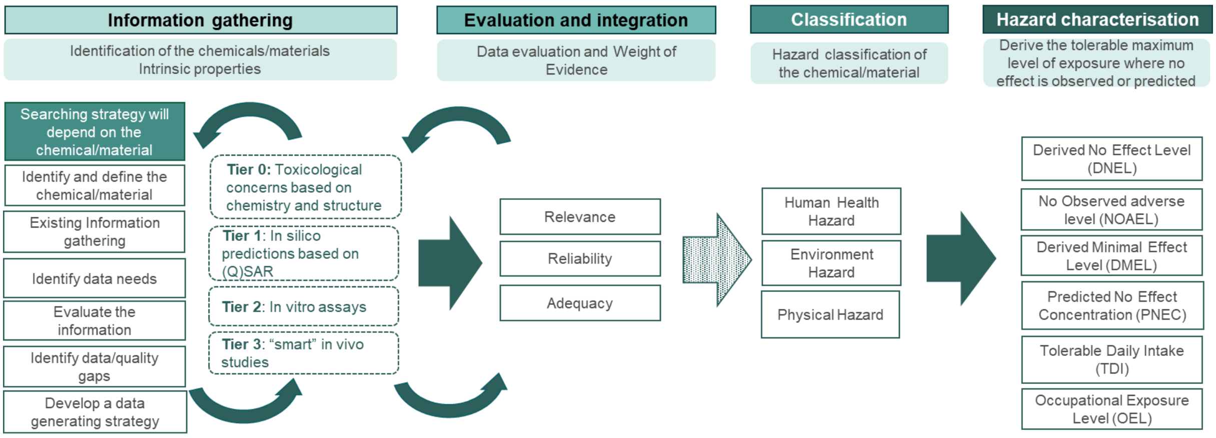
It is not always necessary to derive DNELs for every human population or exposure route or exposure duration. Depending on the exposure pattern and health effects, only relevant DNELs have to be derived. For many local effects (e.g. irritation), DNELs cannot be derived. This may also be the case, for example, for non-threshold mutagens / carcinogens where no safe threshold level can be obtained. In these cases a semi-quantitative value, known as the DMEL or Derived Minimal Effect Level may be developed. Similarly, the PNEC is the maximum level above which a particular environmental compartment (e.g. soil, water, air) should not be exposed. The DNELs are calculated from the toxicological dose descriptors applying an assessment factor. Since dose descriptors are usually obtained from animal studies, an assessment factor is required to allow extrapolation to real human exposure situations and to consider uncertainties.

Other type of exposure threshold levels for specific product applications life the Tolerable Daily Intake (TDI) are also derived from these toxicological dose-response descriptors.

The occupational exposure limits (OELs) are other types of maximum levels above which, in this case, workers should not be exposed and that can be used for Risk Assessment purposes for existing chemicals for which these levels have been established. OELs are established at EU and national level and are typically derived by independent scientific expert committees which consider available scientific information; they are complemented by information on exposure monitoring, such as sampling methodology, measurement methods and measurement systems. OELs are not available for all chemicals and materials.

In the risk characterisation these values (DNEL, PNEC, OEL) are compared against the measured exposure (if existing) or predicted exposure concentrations based on the fate properties and the exposure scenarios. For processes, historical equipment failure data forms the basis for predicting failure rates of specific processes.

Figure 17. Hazard assessment tiered approach.



Source: Own elaboration

Risk characterisation

The risk characterisation establishes the probability of the adverse effect occurring based on the likelihood of exposure. It is characterised as a combination of the chemical/material hazards characterisation and the exposure assessment to the human health and the environment, and it is expressed as Risk Characterisation Ratio (RCR). The RCR is calculated for each relevant exposure pattern (population / compartment, route, and duration of exposure) and each relevant health effect (local and systemic effects).

Human Health: RCR = Measured or predicted exposure concentration / DNEL or

RCR = Measured or predicted exposure concentration / DMEL or

RCR = Measured or predicted exposure concentration / OEL

Environment: RCR = Predicted Environmental Concentration (PEC) / PNEC

The results of the RCR can be:

- If the RCR < 1 the exposure levels are lower compared to the no-effect levels for the relevant time and spatial scales for each of the protection targets: occupational, consumer and environment (OEL, DNEL, DMEL, PNEC). Hence it demonstrates that the risk is controlled.
- If the RCR ≥ 1 the risk is/cannot be controlled, and further actions need to be taken to ensure that the risk is controlled

An SSbD practitioner assessing safety in the context of an SSbD approach can build additional criteria, based on the RCR, for the applicable protection target and exposure routes for the purpose of self-evaluation/conformity (Table 9).

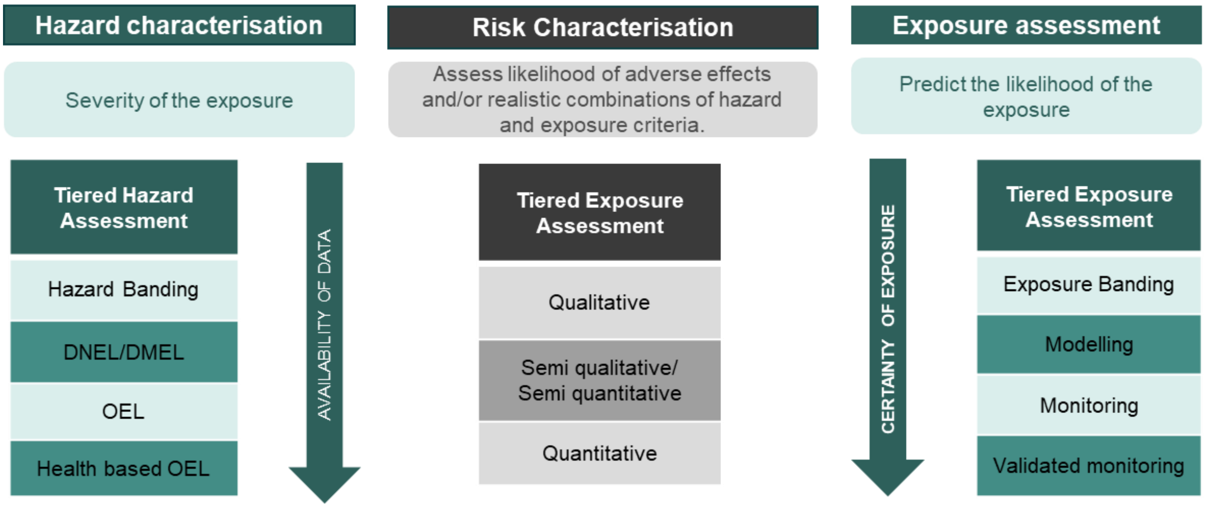
Table 9. Examples of additional criteria that the practitioner could consider depending on the type of innovation and the ambition.

Examples of additional criteria	**SSbD application**
RCR < 1	Cases where SSbD is applied to ensure safety (i.e. safety assessment of an existing SSbD system or breakthrough innovation)
New RCR < current RCR	Cases where SSbD is applied in the (re)design to improve current system's safety (incremental innovation)
New RCR < best RCR	Cases where SSbD is applied in the (re)design to be the best safety option (incremental and breakthrough innovation)

Source: Own elaboration

The risk characterisation is performed in a tiered approach from a qualitative to a quantitative assessment as information both for the hazard and the exposure become available (Figure 18).

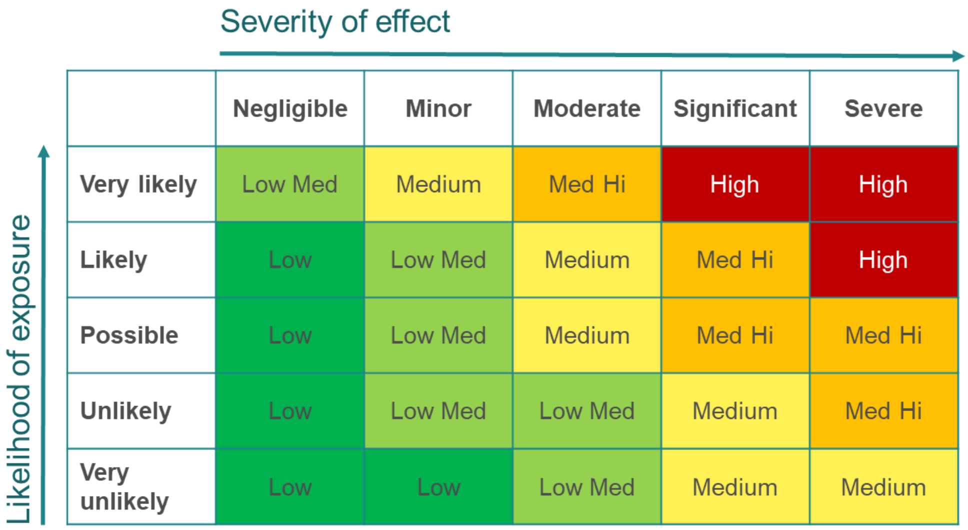
Figure 18. Risk characterisation tiered (qualitative, semi quantitative, quantitative) approach.



Source: Own elaboration

When full data sets are lacking, simplified models (e.g., control banding) can be used to perform a qualitative assessment. These models vary in detail and conservatism but support early-stage decisions. Figure 19 is an example of this so-called control banding approach. Based on the likelihood of the exposure to take place and the severity of the effect different Risk levels are assigned (High, Medium-High, Medium, Low-Medium and Low). Risk level= likelihood of exposure X severity of effect.

Figure 19. Control banding Risk Matrix.



	Negligible	Minor	Moderate	Significant	Severe
Very likely	Low Med	Medium	Med Hi	High	High
Likely	Low	Low Med	Medium	Med Hi	High
Possible	Low	Low Med	Medium	Med Hi	Med Hi
Unlikely	Low	Low Med	Low Med	Medium	Med Hi
Very unlikely	Low	Low	Low Med	Medium	Medium

Source: Adapted from (*Risk Assessment Software* | *RiskPal*.)

Quantitative methods are based on the RCR in a tiered approach based on the exposure scenarios building and quality of data. In Tier 1, exposure is assessed using worst-case assumptions to quickly identify red flags. This tier is intentionally conservative and requires minimal input data (e.g. default values, generic use scenarios). If no risk is identified, the assessment may stop here.

If RCR ≥ 1 the assessment moves to Tier 2, where more realistic use conditions and risk management measures, refined models, and measured or scenario-specific data are incorporated (real concentrations, frequency of use, or site-specific release factors).

Tier 3 involves the highest level of refinement, often using quantitative monitoring data, advanced exposure modelling, and occupational/environmental measurements.

10.3. Uncertainty considerations in Safety assessment

Uncertainty is inherent in all components of safety assessment—problem formulation, chemical/material characterisation, hazard identification, hazard characterisation, exposure assessment, and risk characterisation (Figure 20) and uncertainty in safety assessment combines uncertainties of all individual components Each involves deriving or estimating parameters, values, assumptions, and qualities that reflect the chemical/materials ‘nature and use. This includes intrinsic properties, exposure estimates, and risk levels, all of which carry uncertainties due to data quality, methods used, or model assumptions.

Figure 20. Uncertainties in Safety assessment.

Source: Own elaboration

Uncertainties in the overall **safety assessment** arise from the integration of information from hazard and exposure assessments and from the assumptions, models, and data used throughout the process. These include uncertainties about the representativeness and completeness of available data, the appropriateness of default values or assessment factors, and the cumulative impact of multiple uncertainties on final risk conclusions. Decisions made under limited or evolving data—common in early innovation phases—can introduce systemic uncertainty. It is essential to address these through structured uncertainty analysis, sensitivity analysis, and transparent documentation of assumptions and data sources.

Uncertainties can emerge as early as the **problem formulation**. At this point, incomplete information about the chemical/material, its intended use, life cycle, or potential alternatives can limit clarity in framing the assessment. These uncertainties can lead to wrong assumptions and definition of the system boundaries, misdirected data collection or misinterpretation of risk. To address them, it is essential to ensure early and continuous engagement with life cycle actors, apply a transparent and iterative scoping analysis, and revisit problem formulation as more information becomes available. Documenting all assumptions and rationale clearly from the beginning supports flexibility and transparency throughout the assessment.

Uncertainties in **chemical and material characterisation** derive from limitations in understanding the composition, structure, properties, and behaviour of the chemical or material under assessment. This includes for example variability in: composition of multicomponent chemicals (e.g. UVCB substances), purity, presence of impurities or by-products, particle size distribution (especially for nanomaterials), and stability under different conditions. Inconsistent identification or insufficient characterisation can lead to mismatches between the material tested and the material used in real-world applications, affecting the reliability of the hazard and exposure assessments. Where full characterisation is not possible, conservative assumptions and clear documentation of uncertainties are essential.

In **hazard identification**, uncertainties arise from test data and methods, sample quality, and use of alternative or predictive models. Especially in early innovation stages or with new chemicals/materials, data may be limited. A conservative approach should be applied, using all available information to flag potential hazards. Data quality—accuracy, reliability, completeness and relevance—is critical. In the context of the SSbD also timeliness, i.e. the needed data is available at the relevant point in time, can be also an important attribute, especially at low maturity levels of innovation where rapid screening, red-flag raising is more important that the quality of the data used. These attributes of quality can be weighed differently depending on the innovation maturity. Integrated approaches to testing and assessment (IATAs) can combine multiple data sources to improve predictions and guide further testing.

In **hazard characterisation**, uncertainty may be linked to the choice of test species, endpoints measured, extrapolation between dose levels, or translation from in vitro to in vivo contexts. When data are derived from non-standardised or emerging methodologies, this adds further uncertainty. Additionally, the selection and application of assessment factors (e.g., to derive DNELs or PNECs) introduce judgement-based uncertainty. These factors should be transparently justified, particularly when relying on alternative methods or limited datasets. Data quality again is crucial in reducing uncertainty and supporting robust conclusions.

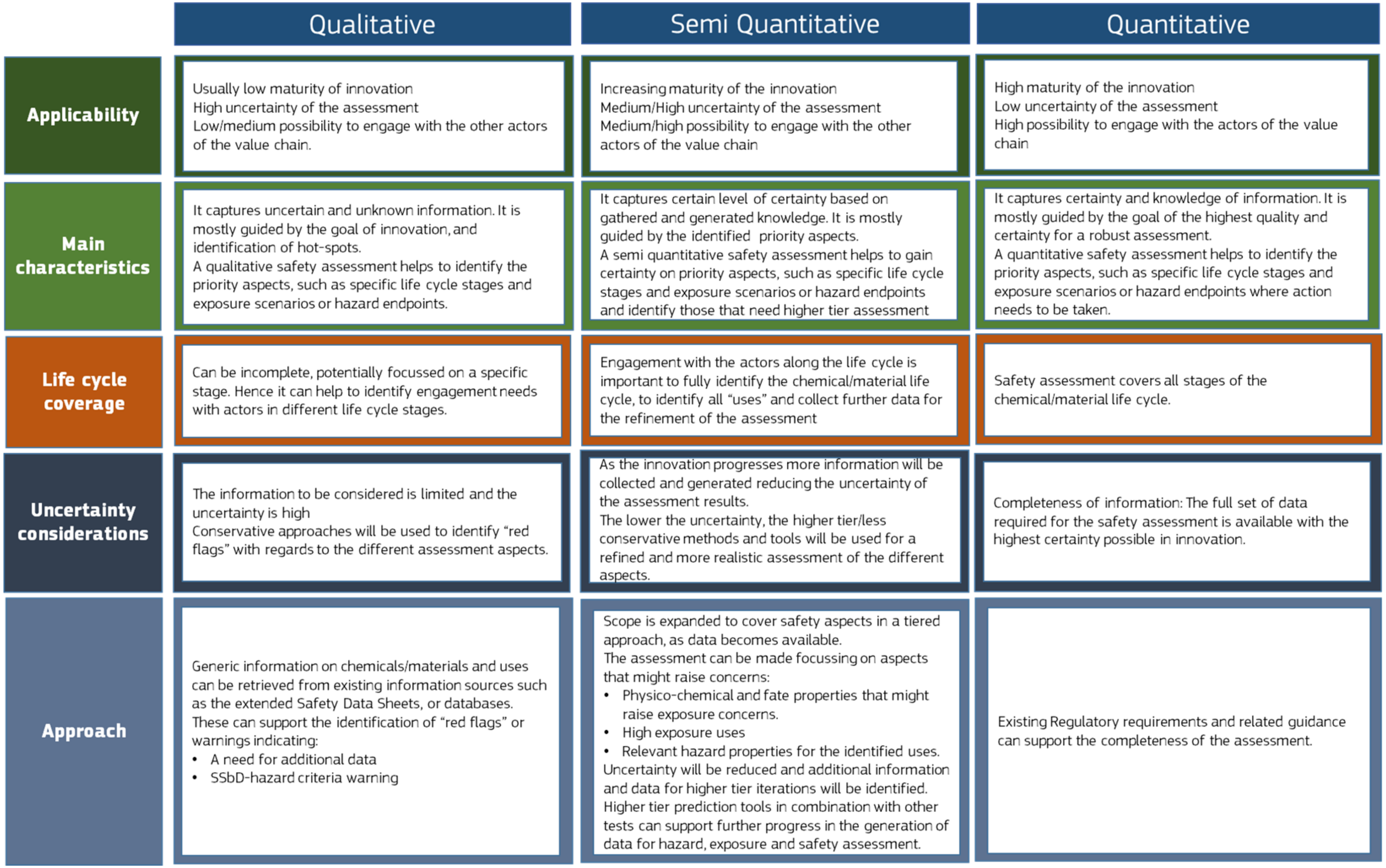
For **exposure assessment**, uncertainty derives from incomplete exposure scenarios, particularly in early innovation. As innovation progresses, knowledge improves. When realistic data is lacking, the use of a **worst-case** or representative scenario is common practice in safety assessment. For transparency and clarity, the selection of the chosen worst-case should always be documented. The World Health Organisation provides guidance for identifying and addressing exposure-related uncertainties. SSbD system definition and life cycle actor engagement is key to shaping exposure assessments.

Risk characterisation is an iterative process that evolves with the accumulation of hazard and exposure data. Uncertainty analysis helps test robustness and identify critical data gaps, guiding efficient data collection. A tiered approach can be taken—from qualitative to quantitative—as data becomes available.

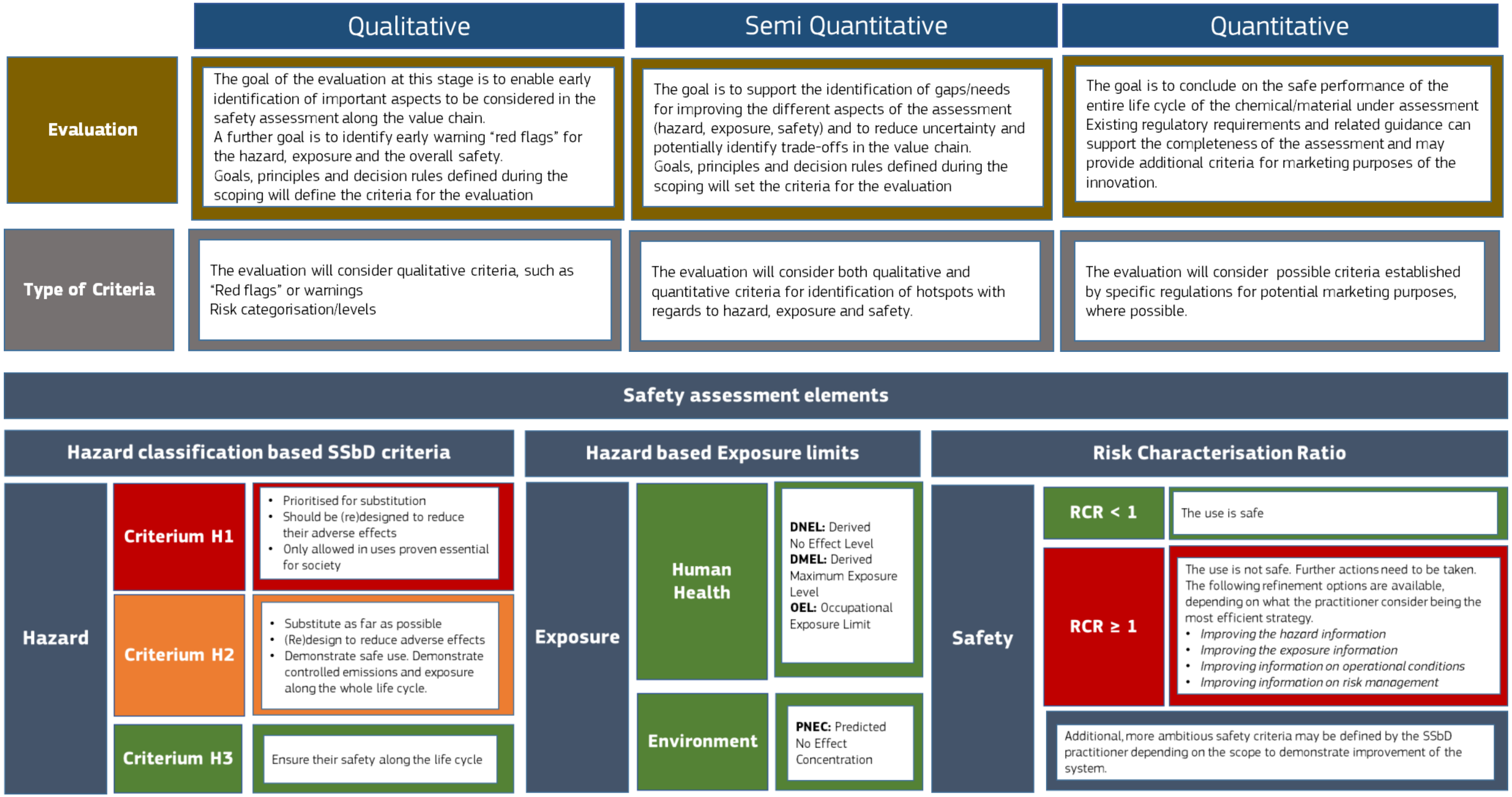
Uncertainty plays a critical role in **comparative assessments**, as these evaluations often involve comparing the safety, of multiple chemicals, materials or products based on diverse and sometimes incomplete data sets. Differences in data quality, availability, and reliability—especially when using alternative methods, including read-across and modelling—can introduce significant uncertainty that affects the outcome of the comparison. If not properly addressed, such uncertainty can result in misleading conclusions about which option is safer. Therefore, transparently identifying, analysing, and communicating uncertainties is essential to ensure that decisions in comparative assessments are robust and scientifically justified.

Figure 21 provides a summary of the qualitative, semi qualitative/quantitative and the quantitative safety assessments based on the aspects, elements and uncertainty considerations described in this chapter.

Figure 21. Tiered approach for the safety assessment.



	Qualitative	Semi Quantitative	Quantitative
Applicability	Usually low maturity of innovation High uncertainty of the assessment Low/medium possibility to engage with the other actors of the value chain.	Increasing maturity of the innovation Medium/High uncertainty of the assessment Medium/high possibility to engage with the other actors of the value chain	High maturity of the innovation Low uncertainty of the assessment High possibility to engage with the actors of the value chain
Main characteristics	It captures uncertain and unknown information. It is mostly guided by the goal of innovation, and identification of hot-spots. A qualitative safety assessment helps to identify the priority aspects, such as specific life cycle stages and exposure scenarios or hazard endpoints.	It captures certain level of certainty based on gathered and generated knowledge. It is mostly guided by the identified priority aspects. A semi quantitative safety assessment helps to gain certainty on priority aspects, such as specific life cycle stages and exposure scenarios or hazard endpoints and identify those that need higher tier assessment	It captures certainty and knowledge of information. It is mostly guided by the goal of the highest quality and certainty for a robust assessment. A quantitative safety assessment helps to identify the priority aspects, such as specific life cycle stages and exposure scenarios or hazard endpoints where action needs to be taken.
Life cycle coverage	Can be incomplete, potentially focussed on a specific stage. Hence it can help to identify engagement needs with actors in different life cycle stages.	Engagement with the actors along the life cycle is important to fully identify the chemical/material life cycle, to identify all "uses" and collect further data for the refinement of the assessment	Safety assessment covers all stages of the chemical/material life cycle.
Uncertainty considerations	The information to be considered is limited and the uncertainty is high Conservative approaches will be used to identify "red flags" with regards to the different assessment aspects.	As the innovation progresses more information will be collected and generated reducing the uncertainty of the assessment results. The lower the uncertainty, the higher tier/less conservative methods and tools will be used for a refined and more realistic assessment of the different aspects.	Completeness of information: The full set of data required for the safety assessment is available with the highest certainty possible in innovation.
Approach	Generic information on chemicals/materials and uses can be retrieved from existing information sources such as the extended Safety Data Sheets, or databases. These can support the identification of "red flags" or warnings indicating: • A need for additional data • SSbD-hazard criteria warning	Scope is expanded to cover safety aspects in a tiered approach, as data becomes available. The assessment can be made focussing on aspects that might raise concerns: • Physico-chemical and fate properties that might raise exposure concerns. • High exposure uses • Relevant hazard properties for the identified uses. Uncertainty will be reduced and additional information and data for higher tier iterations will be identified. Higher tier prediction tools in combination with other tests can support further progress in the generation of data for hazard, exposure and safety assessment.	Existing Regulatory requirements and related guidance can support the completeness of the assessment.



	Qualitative	Semi Quantitative	Quantitative
Evaluation	The goal of the evaluation at this stage is to enable early identification of important aspects to be considered in the safety assessment along the value chain. A further goal is to identify early warning "red flags" for the hazard, exposure and the overall safety. Goals, principles and decision rules defined during the scoping will define the criteria for the evaluation	The goal is to support the identification of gaps/needs for improving the different aspects of the assessment (hazard, exposure, safety) and to reduce uncertainty and potentially identify trade-offs in the value chain. Goals, principles and decision rules defined during the scoping will set the criteria for the evaluation	The goal is to conclude on the safe performance of the entire life cycle of the chemical/material under assessment Existing regulatory requirements and related guidance can support the completeness of the assessment and may provide additional criteria for marketing purposes of the innovation.
Type of Criteria	The evaluation will consider qualitative criteria, such as "Red flags" or warnings Risk categorisation/levels	The evaluation will consider both qualitative and quantitative criteria for identification of hotspots with regards to hazard, exposure and safety.	The evaluation will consider possible criteria established by specific regulations for potential marketing purposes, where possible.

Safety assessment elements

Hazard classification based SSbD criteria

Hazard

Criterium H1
- Prioritised for substitution
- Should be (re)designed to reduce their adverse effects
- Only allowed in uses proven essential for society

Criterium H2
- Substitute as far as possible
- (Re)design to reduce adverse effects
- Demonstrate safe use. Demonstrate controlled emissions and exposure along the whole life cycle.

Criterium H3

Ensure their safety along the life cycle

Hazard based Exposure limits

Exposure

Human Health

DNEL: Derived No Effect Level
DMEL: Derived Maximum Exposure Level
OEL: Occupational Exposure Limit

Environment

PNEC: Predicted No Effect Concentration

Risk Characterisation Ratio

Safety

RCR < 1

The use is safe

RCR ≥ 1

The use is not safe. Further actions need to be taken. The following refinement options are available, depending on what the practitioner consider being the most efficient strategy.
- *Improving the hazard information*
- *Improving the exposure information*
- *Improving information on operational conditions*
- *Improving information on risk management*

Additional, more ambitious safety criteria may be defined by the SSbD practitioner depending on the scope to demonstrate improvement of the system.

Source: Own elaboration

10.4. Process-related safety

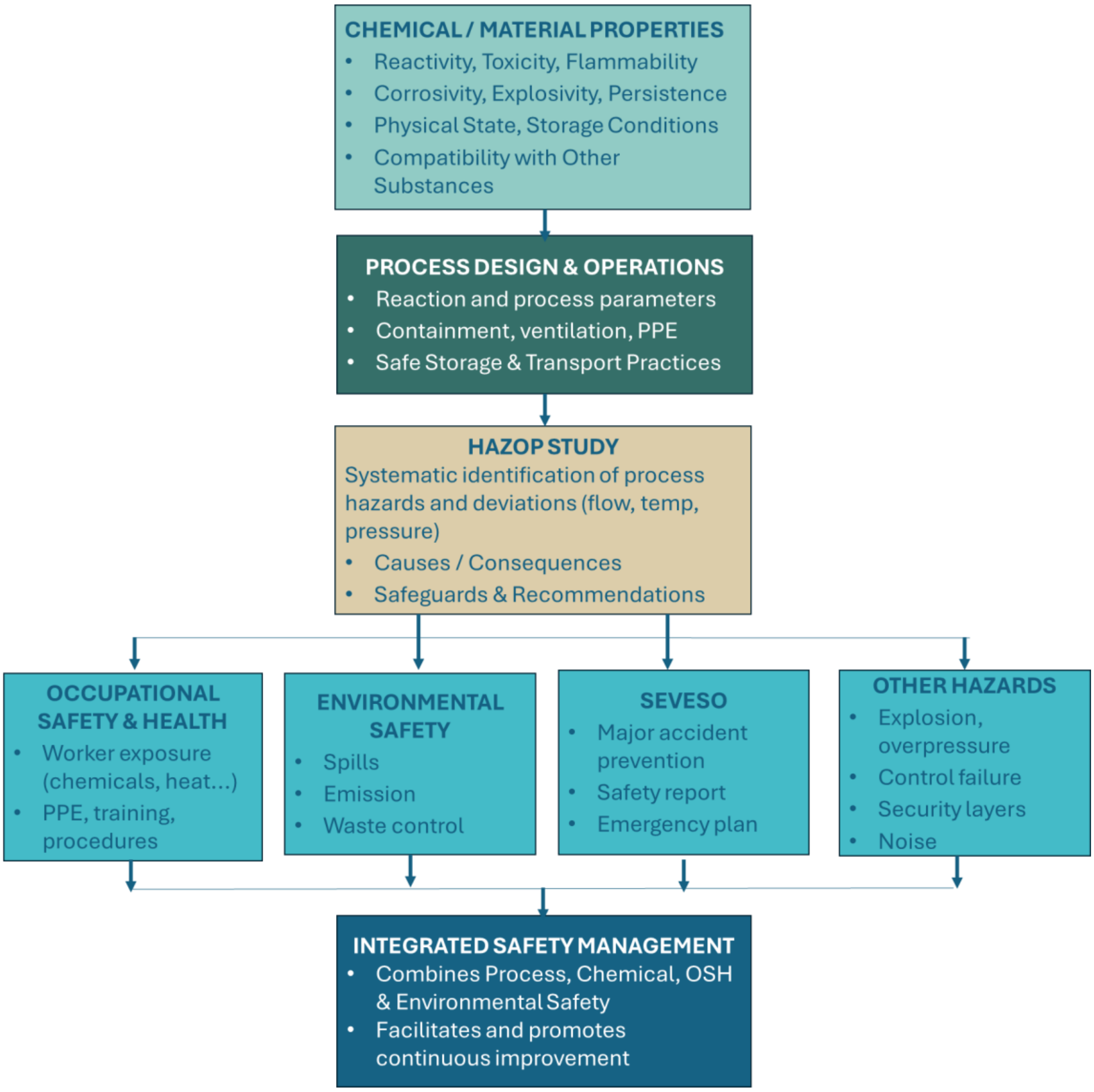
Chemical safety focuses on the identification of the hazard properties of the chemical/material and the estimation of the risks associated with the exposure along its entire life cycle, for both human and environment. Normally this includes many safety considerations associated with the particular process; for manufacturing of a chemical or material, the properties of the chemical, its precursors, residual waste and specific operational conditions associated with the technology employed are all necessary to consider in the assessment and as necessary address/mitigate any associated risks.

The life cycle stages can also be assessed by themselves, to identify and integrate any aspects related to the protection of human health and the environment that are not directly associated to the manufactured chemical or material and may have been missed. A holistic approach to SSbD safety assessment expects consideration and integration of any such further process-related safety aspects.

Process-related safety can be considered for the use of the chemical/material (e.g. manufacturing plant) and the end-of-life stage (e.g. waste management operations, including recycling, recovery and disposal (EC, 2008b). One relevant aspect here is that by applying a holistic perspective we can identify safety issues not identified when assessing the chemical/material like for example safety issues related to the alternative manufacturing processes (for example, a biotechnological process) (Nakhal Akel et al., 2025; Wessberg et al., 2008).

By incorporating elements that focusses on process/technological hazard and risk, SSbD practitioners can better align safety objectives along the innovation of the process design (as reported in the Figure 22 below).

Figure 22. Process safety scheme.



Source: Own elaboration

The assessment of process-related safety starts with the scoping analysis and the identification of the chemical/materials used and their properties together the relevant processes activities (Figure 22). Through the scoping analysis the different elements can be identified regarding the process e.g. the precursors, process conditions, and operational parameters involved throughout the production lifecycle, such as auxiliary materials (e.g. solvents, catalysts), and specific operating conditions (e.g. high pressure, elevated temperature, exothermic reactions). The chemical safety aspects are already covered in sections 10.1, 10.2. and 10.3. However, process safety integrates other safety considerations to ensure the protection of human health and environment[6], and these elements needs to be assessed as well[7].

From this perspective, a process safety assessment can combine the chemical hazard identification with assessment of risks of the 'hardware', i.e. the production facility. It focuses on preventing equipment failure in facilities that use, process, storage and handle hazardous chemicals/materials. It addresses the design, operation, maintenance, and management of chemical processes to avoid fires, explosions, accidental chemical releases. These equipment failure risks are especially pertinent in chemical process development and should be considered from the earliest stages of technological innovation, onwards.

A HAZOP (Hazard and Operability Study) is a structured approach used to examine how deviations from the intended process design can lead to hazardous situations or operational issues. It analyses the causes by identifying the hazards that could harm workers, equipment, or the environment and operability problems that might cause plant shutdowns or product quality issues. It evaluates the adequacy of existing safeguards (alarms, interlocks, relief systems) and it recommends actions to eliminate or reduce risks. It's typically performed during the design phase of a new process (or when modifying an existing one) and is often required by safety regulations (IEC, 2016).

HAZOP expands risk coverage beyond chemical/operational aspects and includes mechanical, control, fire, and explosion hazards linked to process deviations. Biological agents like bacteria, fungi, or their toxins (e.g. endotoxins, mycotoxins) can introduce additional layers of complexity to process safety. Improper handling, temperature fluctuations, or waste accumulation can lead to microbial contamination, pressure build-up, or even biogas explosions. Specific indicators related to these risks can be included in the process design, such as on the efficiency of sterilisation systems in place or on unintended release of biological material.

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[6] It should be noted that the exposure to a single, pure chemical does not exist in the real world, instead the chemical pollution is characterised by complex multi-component mixtures that can easily comprise dozens or even hundreds of chemicals (Bopp et al., 2015).

[7] This approach is also aligned with the Chemicals Management System and chemicals inventories foresees by Art. 14a of the Industrial Emissions Directive (EC, 2024b) that emphases reducing chemical and process risk at source by virtue of moving towards less intrinsically hazardous chemicals, and also via reducing the volumes/ masses present and used in reactions onsite.

The identification of hazards and risks hotspots, as related to processes and operations, goes beyond the exposure to chemical(s) and includes, among others, the exposure to physical and biological agents[8]. HAZOP supports OSH (Occupational Safety and Health) by identifying risks from process deviations (e.g., leaks, overpressure…). Supports worker protection programs, PPE selection, and training.

A HAZOP study feeds into the environmental risk assessments by identifying and analysing potential pathways through which industrial processes could impact air, water, and soil compartments. It bridges process safety and environmental protection by identifying, assessing, and mitigating all routes to potential pollution. A HAZOP study detects how process deviations could lead to leaks, spills, or emissions (e.g., valve failure, overpressure venting, thermal runaway) causing harm to ecosystems and natural habitat. These findings can provide essential input, for example, to the Environmental Management System (EMS) under the Industrial Emissions Directive (IED), ensuring process integrity and environmental protection.

Risk arising from accidental releases should be also considered[9]. HAZOP results are used as input for hazard identification and Safety Report documentation contribute to SEVESO compliance for prevention and mitigation of major accidents.

The integrated safety management combines and manages all safety aspects under one system. It provides traceability and compliance assurance across the life cycle and ensures continuous monitoring and improvement.

The process safety can be performed in a tiered approach. At low innovation maturity levels, completeness and quality of the information/data, precise information about tonnages, storage conditions, and full-scale process parameters is generally not available. However, the early design phase offers the most effective opportunity to embed safety principles. Implementing a process-oriented risk evaluation at this stage can support the identification and prioritisation of safer process alternatives. An example of screening of process related safety is reported in Box 10.

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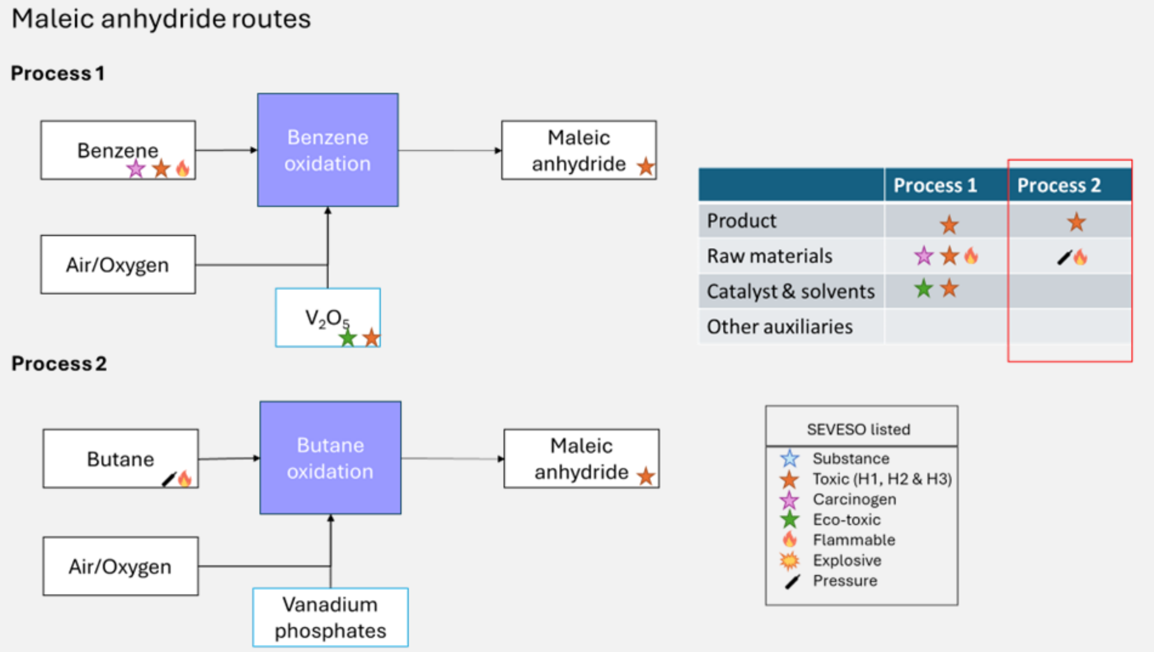
[8] The way in which these risks are identified and indicators are built, can leverage on the existing procedures for risk evaluations such has the HAZOP (Hazard and Operability) which is a structured and systematic approach use to identify potential hazards and operability problems in complex systems and processes.

[9] Such as the Directive (EU) 2012/18, the Seveso III Directive on the prevention of major accidents, and reduction of associated hazards and risks involving dangerous substances, or the (EU) Directive 2009/41 on the contained use of genetically modified micro-organisms.

Box 10. Screening of process-related safety at early stage of process development.

The same chemical or material, having the same hazard profile, might lead to significant differences in the overall safety assessment when produced using different feedstocks or by means of different production processes. And for that reason, process (re)design plays an important role in the context of the SSbD.

For example, the figure below presents a comparison between two manufacturing processes to produce maleic anhydride. Historically, maleic anhydride was primarily produced by the catalytic oxidation of benzene (Lohbeck et al, 2000). Today, the preferred industrial process for producing maleic anhydride is the catalytic oxidation of n-butane. Using the basic information available already at early stage (i.e. raw materials, catalyst and possible operating conditions) the two processes can be compared to identify red flags to understand which process pose more risk at plant-level.



Source: Own elaboration

Avoiding hazardous precursors might be an improvement of the process from the safety perspective but if generates large volumes of difficult-to-treat waste downstream, its overall environmental benefit diminishes. Similarly, one process might seem more efficient than the other, but if it uses highly hazardous raw materials, or if its byproducts pose long-term environmental hazards, this may represent, potentially, an unacceptable trade-off.

By assessing chemical processes in their entirety, we can identify hidden environmental burdens and potential risks that would otherwise be missed. This holistic approach includes:

- Risk Management: Identifying and addressing potential hazards associated with raw materials, auxiliary materials, products, and waste streams in early innovation
- Optimisation: Finding the most sustainable pathways by minimising impact across the entire value chain.

The safety assessment of the process reduces the likelihood of industrial impact and accidents and fosters a safety culture where prevention is built into innovation, ensuring that new technologies are both effective and aligned with long-term sustainability goals. To ensure the operational effectiveness of this approach, it is essential that practitioners implement qualitative and quantitative indicators and assessment criteria tailored to the specific context to cover, as far as possible, the relevant sources of risk.

A systematic assessment of potential hazards, including component failure, and the implementation of appropriate risk reduction measures can lead to better pricing of risk. This is fundamental to access to credit and reduce its cost as well as cost of insurance. Thus, early integration of risk evaluation supports both operational resilience and cost-effective capital management, affecting chemical industries overall competitiveness.

Incorporating safety assessment into process development not only enhances safety and regulatory compliance but also contributes to financial stability and resilience.

11. Environmental sustainability assessment

The **environmental sustainability of chemicals and materials** is performed by means of Life Cycle Assessment (LCA), to identify hotspots along the life cycle of the chemical/material and to steer the innovation towards feedstock and processes that could minimize the environmental footprint. Indeed, when SSbD design principles are applied, including those that are expected to improve the overall sustainability of the innovation, the resulting innovation should be assessed in terms of the sustainability performance, identifying as early as possible, hotspot of impacts and trade-offs to be minimised.

The environmental sustainability assessment within the SSbD context can only be performed if the intended use(s) is considered. Therefore, a function-based LCA including the entire life cycle must be conducted. It is recommended to conduct the LCA following the existing EC guidelines[10].

Nevertheless, a **tiered approach** for the LCA is here introduced and described to support the assessment of the environmental impact assessment throughout the innovation of the chemical/material – also when the intended use(s) is unknown or undefined. In all cases, the LCA results should be presented stating clearly the assumptions and data sources used.

The following chapters address:

- Aspects, indicators and criteria to consider
- Assessment and evaluation system throughout the innovation

11.1. Aspects, criteria and indicators

Environmental sustainability embraces a variety of different aspects[11]. Some aspects are widely modelled, such as those translated into the impact categories considered in the Environmental Footprint (EF) Impact assessment method with the respective indicators[12] (current version EF3.1.). Figure 23 shows those indicators from the EF and included in the SSbD framework corresponding to the total 16 impact categories that are related to several policy objectives such as protection of human health and of biodiversity. Other aspects (e.g. environmental impact due to release of microplastics) can be further integrated into future LCA practices and might need to be addressed on a case-by-case basis by the criteria developer, addressing possible indicators and ranges.

It is important to note that the aspects are interlinked as, for example, pollution and climate change are key drivers of impacts on biodiversity loss and human health.

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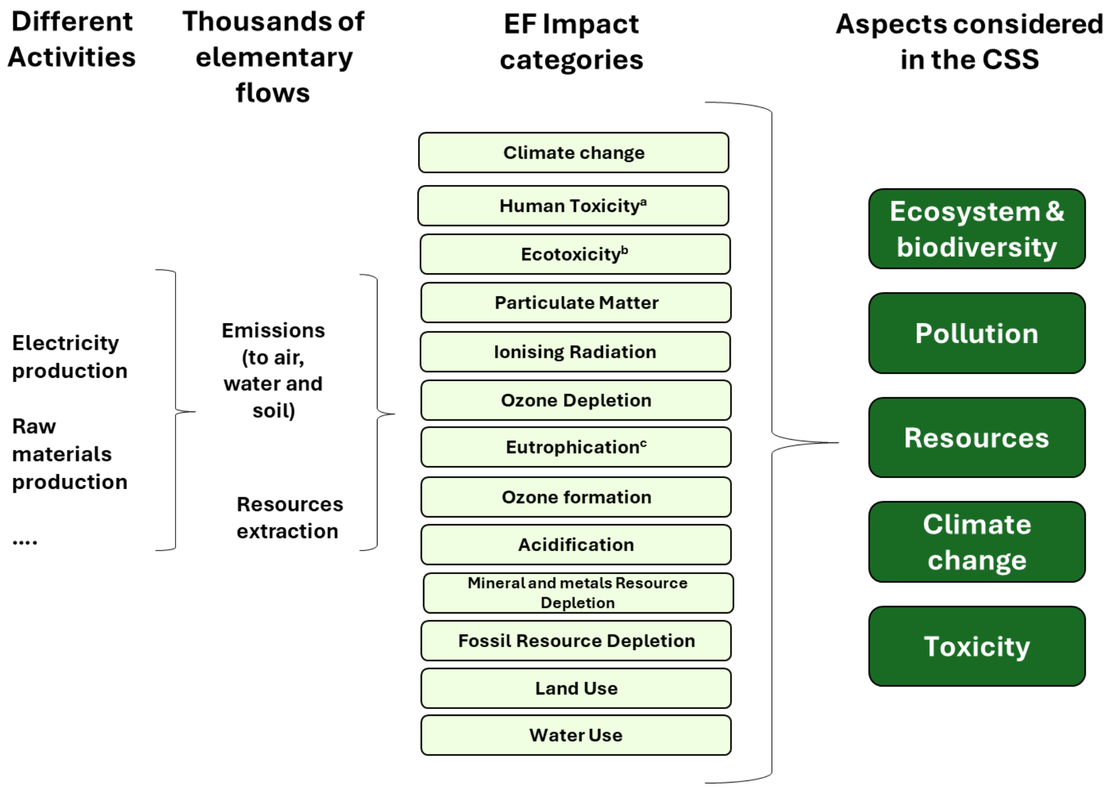
[10] It is recommended to refer to existing EC guidelines, i.e. the Product Environmental Footprint (PEF) method (EC, 2021b), which is the European Commission recommended method to assess the life cycle environmental performance of products on the market. The method is inspired by the ISO 14040 and 14044 (ISO, 2006, 2020) standards and it is providing further guidance and requirements to ensure the replicability and comparability of the LCA results, at the level of data (format and nomenclature), modelling principles for inventories, impact assessment methods and related characterisation factors, normalisation, and weighting. Moreover, it provides general rules for multi-functional process (i.e., processes that produce more than one valuable output).

[11] See e.g. the taxonomy of impacts proposed by (Bare & Gloria, 2008).

[12] This method is recommended by the European Commission for the LCA of products (EC, 2021b) and could be considered as a minimum set of impacts to be addressed when conducting an LCA study.

The EF 3.1 method (Andreasi Bassi et al., 2023) includes human toxicity (cancer and non-cancer) and ecotoxicity impact, which refer to impacts due to all chemicals being emitted along the product life cycle, which ultimately may impact humans and the environment via environmental compartments (e.g. soil, water, air). The focus of the human toxicity and ecotoxicity impact assessment is on the indirect impacts via different compartments and on the overall toxicity footprint, rather than a specific focus on direct exposure which differ from the aspects covered in the safety assessment (chapter 10).

Figure 23. Environmental Footprint (EF) impact categories, and their link to key issues considered in the Chemicals Strategy for Sustainability (CSS).



Source: Own elaboration adapted from Caldeira et al. 2022b

Toxicity and ecotoxicity impact categories also relate to pollution. Aside from the three impact categories related to toxicity, the EF method includes 13 additional impact categories, providing a broader view on the overall life cycle environmental impact. The 16 impact categories relate to the CSS objective of minimising the environmental footprint of chemicals, in particular regarding climate change, resource use, ecosystems and biodiversity (Figure 23). A short description of each impact category covered in the EF method is provided in Annex 5.

The 16 impact categories result from modelling the life cycle of the chemical, from raw material extraction up to the end of life. The impacts result from the multiplication of the emissions and resources used along the life cycle as well as of the chemicals in the given material/product application (elementary flows /pressures[13]) by the characterisation factors (CFs) associated to each of them. The 16 indicators may optionally also be expressed also as a single score, as part of the EF method. However, it is suggested retaining the 16 individual indicators for fuller reporting, to better illustrate the potential trade-offs between them, taking into account the main hotspots.

The impact categories included in the SSbD Framework may be subject to updates, following updates in the EF method. These updates refer to the continuous future advancement of LCA, via including additional, or refined impact categories. For instance, presently, there is not a fully agreed impact category in the EF method which addresses biodiversity loss. Nevertheless, the EF method accounts for the main drivers for biodiversity loss, such as Climate Change or Land Use. Hence, EF results could be considered a proxy of a "biodiversity footprint" via the means of evaluating the above-mentioned underpinning drivers of loss. It should be noted that several Life Cycle Impact Assessment (LCIA) methods to estimate impacts on biodiversity have been developed, however[14].

In the EF Life Cycle Impact Assessment (LCIA), the characterized results undergo a normalization step and, optionally, a weighting step.[15] The weighted impact categories can then be summed to obtain the EF single overall score (Andreasi Bassi et al., 2023). These steps support the interpretation (e.g. identification of hot-spots and dealing with trade-offs among impact categories) and communication of the results of the analysis.

Within the SSbD context, it is suggested that the impact categories are addressed separately at characterization level to enhance the **identification of hot spots** and area for improvement. Optionally, the practitioner could decide to consider the normalization and weighting steps, up to the single overall score, when deemed applicable. (see section 11.2 for more details on the results interpretation).

Aspects and indicators are accompanied by the definition of **criteria** to support the interpretation of the LCA results. The criteria serve to guide the innovation by providing ***reference* values** – such as thresholds or targets – that enable comparative assessment to determine how the innovation is performing with respect to the environmental sustainability.

Expanding and adjusting the definition provided by the PEF Recommendation the SSbD studies could consider a *reference*[16], against which comparisons with the performance (e.g. impact result from LCA application) of the chemical under assessment could be made, to support inputs to the process of decision making.

Such a *reference* cannot be unique and fixed for all types and instances of SSbD implementation, since the comparison is performed for the functional unit (and this varies according to the specific

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[13] (Environmental) Pressures are all emissions (to air, water, and soil), resource use (minerals, fossil fuel, renewables) as well as physical emissions such as noise and radiation resulting from human activity (Caldeira et al., 2022b).

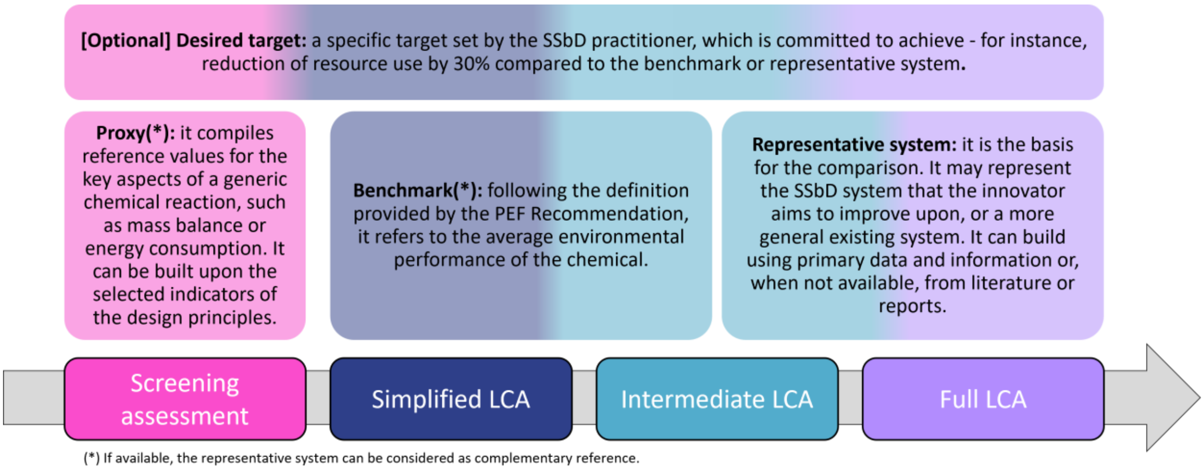
[14] IMPACTworld (Bulle et al, 2019), LC-IMPACT (Verones et al., 2020) or ReCipe2016 (Huijbregts et al., 2017)) that are being assessed to be used in the context of the EF method.

[15] In the normalization, the results are divided by the overall inventory of a reference unit, e.g., the entire world, to convert them in relative shares of the impacts of the analysed system. In the weighting, each impact category is multiplied by a weighting factor to reflect their perceived relative importance (Andreasi Bassi et al., 2023).

[16] The reference for an LCA study has been already introduced and defined in the PEF Recommendation, and the PEF nomenclature is to call it a "Benchmark", referring to *"the average environmental performance of the representative product sold in the EU market"*. The representative product is a real or virtual (non-existing) product. The virtual product should be calculated based on average European market sales-weighted characteristics for all existing technologies/materials covered by the product category or sub-category (EC, 2021b).

application / context). Moreover, the *reference* evolves throughout the implementation of the SSbD framework, in accordance with the iterative and tiered approach of the SSbD framework. Figure 24 illustrates the various *references* for the environmental sustainability assessment along with the related definitions and where – along the innovation – it is more suitable to be defined. Note that there can be situations where the representative system can be used as reference already at the early stage of innovation.

Figure 24. Reference for the environmental sustainability assessment along the innovation of the chemical/material.



[Optional] Desired target: a specific target set by the SSbD practitioner, which is committed to achieve - for instance, reduction of resource use by 30% compared to the benchmark or representative system.

Proxy(*): it compiles reference values for the key aspects of a generic chemical reaction, such as mass balance or energy consumption. It can be built upon the selected indicators of the design principles.

Benchmark(*): following the definition provided by the PEF Recommendation, it refers to the average environmental performance of the chemical.

Representative system: it is the basis for the comparison. It may represent the SSbD system that the innovator aims to improve upon, or a more general existing system. It can build using primary data and information or, when not available, from literature or reports.

(*) If available, the representative system can be considered as complementary reference.

Source: Own elaboration

Once the *reference* is defined, the related **classes of performance** of the innovation are identified (Table 10). Each class of performance potentially comprise upper and lower limit values delimiting a range of e.g. reference LCA impacts. This enables the practitioner to assess how good or bad the LCA results of the chemical under assessment are compared to the reference. A **score** can be subsequently assigned to each class of performance to simplify the interpretation of the results and visualisation. Further details regarding the range of values for the benchmark and proxy reference are reported in sections 11.1.1 and 11.1.2.

Based on the classes of performances, it is then possible to compare the obtained results of the chemical under assessment against the defined reference (Table 10). As shown in the Figure 25, the classes of performances can be built differently according to the choice of the practitioner. In the example, the classes of performances in the case of the proxy/benchmark are defined according to quartiles and maximum value of a set of average impact results (see sections 11.1.1 and 11.1.2 for more details), and the representative system are defined according to a selected level of improvement.

Table 10. Criteria and scores to be applied to the LCA result of the chemical under assessment for each impact category, according to the reference identified.

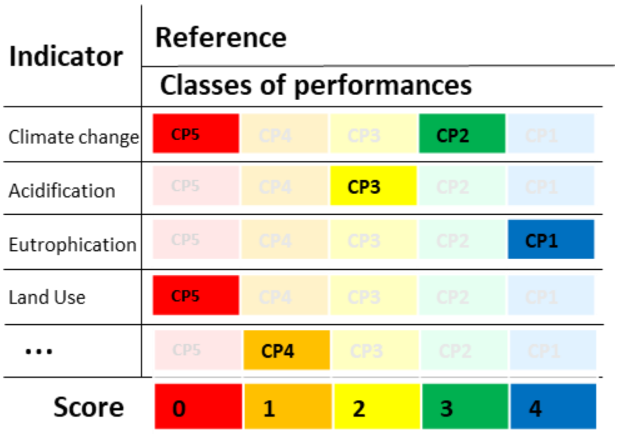
Range of values Benchmark [1]	Representative system	Score	Class of performance [2]	
LCA result > maximum value	No improvement / Worsening	0	CP5	Fail the criteria
LCA result > Q3	Improvement + 5%	1	CP4	
Q2 < LCA result ≤ Q3	Improvement + 5% to 20%	2	CP3	Pass the criteria
Q1 < LCA result ≤ Q2	Improvement + 20% to 40%	3	CP2	
LCA result ≤ Q1	Improvement > 40%	4	CP1	

[1] *"Q" means "quartiles", as described in section 11.1.2*

[2] *The identified "classes" are illustrative and should be defined considering the uncertainty of the assessment.*

Source: Own elaboration adapted from (Caldeira et al., 2022b)

Figure 25. Qualitative example of the classes of performance ("CP") and related score for the assigned reference (i.e. proxy reference, benchmark or representative system).



Indicator	Reference Classes of performances				
Climate change	CP5	CP4	CP3	CP2	CP1
Acidification	CP5	CP4	CP3	CP2	CP1
Eutrophication	CP5	CP4	CP3	CP2	CP1
Land Use	CP5	CP4	CP3	CP2	CP1
...	CP5	CP4	CP3	CP2	CP1
Score	0	1	2	3	4

Source: Own elaboration

An example of use of references for the interpretation and evaluation of the results, combining different types of references for medium/high TRL, is reported in Annex 6.

11.1.1.Definition of the "proxy" reference

The **proxy reference** can be used to enable screening assessments of the innovation to preliminarily identify hot-spot and performances of the reaction.

The **proxy refence** provides ranges of values for key indicators representing a general chemical reaction. Ranges of values are derived for the most common indicators of a generic chemical reaction, which are the mass balance and the enthalpy, and calculated based on the stochiometric reaction. The mass balance gives an idea about the efficiency of reaction and potential by-products; the enthalpy gives preliminary information about the energy, either if there is a need for energy supply (i.e. heating or electricity) or if there is a generation of energy (i.e. need for managing this excess of energy). Ranges of values for indicators can help in identifying their actual fulfilment. Table 11 shows an example of ranges of values for the indicators linked to the design principles, retrieved from existing studies on organic chemicals.

Table 11. Examples of ranges of values for the indicators linked to design principles proposed in the SSbD framework.

Code	SSbD principle	Indicator	Best case	Worst case
SSbD1	Material efficiency	Net mass of materials consumed (kg/kg)	1	40%
		Reaction Yield (%)	100%	40%
		Atom Economy (MWproduct/MWtotal reaction)	100%	
		Material Intensity index (kg materials / kg product)	100%	
		Environmental impact factor - E-factor (%) (Input materials - product)/product	0%	
		Recycling of the solvent and purity	99 -100% (purity)	
		Solvent selectivity (kgsolvent/kgproduct)	0%	
		Water consumption (m^3/kg)	0	2.95
		Recycling efficiency/recovery rate (%)	100%	
		Total amount of waste (kg/kg)	0%	
		Amount of waste to landfill (kg/kg)	0%	100%
		Critical Raw Material presence (yes/no + amount)	0%	100%
SSbD2	Minimise the use of hazardous chemicals/materials	Biodegradability of manufactured chemical/Material	100%	0%
		Classification of raw chemicals/materials as SVHC (yes/no + amount)	0%	1 kg/kg
SSbD3	Design for energy efficiency	Energy efficiency (%)	Min. theoretical energy ΔG kJ/kg	1.949x10^6 kJ/kg
		Yield of extraction (mass of recovered solvent / used solvent)	100%	0%
SSbD4	Use renewable sources	Renewable or fossil feedstock (yes/no + amount)	100%	0%
		Recycled content (%)	100%	0%
		Share of Renewable Energy (%)	100%	0%
SSbD5	Prevent and avoid hazardous emissions	Non-Aqueous Liquid Discharge (m^3/kg)	0%	100%
		Wastewater to treatment (m^3/kg)	0%	100%
		Amount of hazardous waste (kg/kg)	0%	1 kg/kg
SSbD6	Reduce exposure to hazardous substances	Biodegradability of manufactured chemical/Material	100%	0%
		Classification of raw chemicals/materials as SVHC (yes/no)	0%	100%
SSbD7	Design for end-of-life	Recyclable? (yes/no)	100%	0%
		Durability (years)		0-1
		Disassembly/reparability design (yes/no)	100%	0
SSbD8	Consider the whole life cycle	Recyclable? (yes/no)	100%	0%
		Disassembly/reparability design (yes/no)	100%	0%
		Material Circularity indicator (MCI)	1	0
		Biodegradability of manufactured chemical/Material	100%	0%

Source: Own elaboration

11.1.2.Definition of the benchmark

The **benchmark** can be used as reference in simplified and intermediate assessment to enable comparison and preliminary decision-making of the innovation. For instance, when assessing a **new chemical / material**, or as an indication of the average environmental performance of existing chemicals / materials, and groups (e.g. belonging to the same "family") of chemicals / materials. The **benchmark** is defined as the *average* impact value for each impact category. Thus, the benchmark does not represent a real chemical but is rather a virtual representative average-impact chemical. To build an initial set of benchmark values to be used in SSbD, a basket of chemicals has been built, starting from the list of large volume organic (and some inorganic) chemicals in the Best Available Techniques (BAT) Reference Document for the Production of Large Volume Organic Chemicals provided by Falcke et al. 2017. The average impact was calculated for the production process ("cradle-to-gate") of 1 kg of the selected chemicals using available LCA databases and the EF 3.1 method (Andreasi Bassi et al., 2023). The average was performed at the level of each chemical, when available in more databases and when different production routes (e.g. feedstock origin) were available. Future benchmark(s) could encompass also "specialties", i.e. low product volume chemicals characterised by their use for specific applications.

Based on the average LCA impact value of selected chemicals, quartiles[17] and the maximum value – are derived, which describe the increasing impact across selected chemicals and, thus, lower sustainability performance.

Ultimately, the five **"classes" of performance -** reported in Table 12 – are derived from the defined benchmark and are used for the comparison of the LCA results of the chemical under assessment. From the classes of performance, it is possible to create **criteria** for the assessment that cover the cradle-to-gate system, as shown in Table 10. In practice, once the LCA results of the production process of 1 kg of the chemical under assessment are calculated, each result is assigned to a class of performance based on the ranges shown in Table 12.

For the remainder of the **life cycle** of the chemical/material, other types of reference need to be defined, on a case-by-case basis.

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[17] The quartiles are three values that divide the set of data in four intervals: Q1 (corresponding to 25th percentile of the set of data), Q2 (corresponding to 50th percentile of the set of data), Q3 (corresponding to 75th percentile of the set of data).

Table 12. Ranges of impact for the 16 impact categories that to define the classes of performances (CPs), against which the impact result for the production of 1 kg of the chemical under assessment should be compared.

Impact category	**Unit**	**CP1**	**CP2**	**CP3**	**CP4**	**CP5**
Acidification	mol $H+_{eq}$	< 6.37e-03	[6.37e-03, 9.61e-03)	[9.61e-03, 1.58e-02)	[1.58e-02, 3.19e-02)	≥ 3.19e-02
Climate change	kg $CO_{2\ eq}$	< 1.97e+00	[1.97e+00, 2.88e+00)	[2.88e+00, 4.50e+00)	[4.50e+00, 9.44e+00)	≥ 9.44e+00
Ecotoxicity, freshwater	CTUe	< 1.38e+01	[1.38e+01, 2.11e+01)	[2.11e+01, 3.84e+01)	[3.84e+01, 2.50e+02)	≥ 2.50e+02
Eutrophication, freshwater	kg P_{eq}	< 1.74e-04	[1.74e-04, 3.60e-04)	[3.60e-04, 6.39e-04)	[6.39e-04, 4.33e-03)	≥ 4.33e-03
Eutrophication, marine	kg N_{eq}	< 7.68e-04	[7.68e-04, 1.47e-03)	[1.47e-03, 2.70e-03)	[2.70e-03, 1.51e-02)	≥ 1.51e-02
Eutrophication, terrestrial	mol N_{eq}	< 1.21e-02	[1.21e-02, 1.72e-02)	[1.72e-02, 3.41e-02)	[3.41e-02, 6.98e-02)	≥ 6.98e-02
Human toxicity, cancer	CTUh	< 3.10e-09	[3.10e-09, 6.36e-09)	[6.36e-09, 1.31e-08)	[1.31e-08, 6.43e-08)	≥ 6.43e-08
Human toxicity, non-cancer	CTUh	< 1.69e-08	[1.69e-08, 2.37e-08)	[2.37e-08, 4.61e-08)	[4.61e-08, 6.42e-07)	≥ 6.42e-07
Ionising radiation, human health	kBq U^{235}	< 5.78e-02	[5.78e-02, 8.95e-02)	[8.95e-02, 1.53e-01)	[1.53e-01, 7.05e-01)	≥ 7.05e-01
Land use	Dimension-less (pt)	< 3.14e+00	[3.14e+00, 4.48e+00)	[4.48e+00, 8.52e+00)	[8.52e+00, 1.13e+02)	≥ 1.13e+02
Ozone depletion	kg CFC-11_{eq}	< 3.44e-08	[3.44e-08, 5.62e-08)	[5.62e-08, 1.11e-07)	[1.11e-07, 5.76e-06)	≥ 5.76e-06
Particulate matter	Disease incidences	< 5.47e-08	[5.47e-08, 9.35e-08)	[9.35e-08, 1.73e-07)	[1.73e-07, 4.82e-07)	≥ 4.82e-07
Photochemical ozone formation, human health	kg $NMVOC_{eq}$	< 8.21e-03	[8.21e-03, 1.00e-02)	[1.00e-02, 1.36e-02)	[1.36e-02, 5.26e-02)	≥ 5.26e-02
Resource use, fossils	MJ	< 5.51e+01	[5.51e+01, 6.85e+01)	[6.85e+01, 8.66e+01)	[8.66e+01, 1.34e+02)	≥ 1.34e+02
Resource use, minerals and metals	kg Sb_{eq}	< 7.50e-06	[7.50e-06, 1.15e-05)	[1.15e-05, 2.33e-05)	[2.33e-05, 9.79e-05)	≥ 9.79e-05
Water use	m^3 world eq. deprived water	< 4.35e-01	[4.35e-01, 1.15e+00)	[1.15e+00, 1.87e+00)	[1.87e+00, 5.50e+00)	≥ 5.50e+00

Source: Own elaboration

11.2. Assessment and evaluation system throughout the innovation

A screening assessment is also considered for very initial SSbD system where it is not possible to perform an LCA. Figure 11 shows the tiered approach for the implementation of the SSbD framework. The top left side of the figure introduces screening assessment when the maturity of the innovation is low, and consequently the information and data are very little.

The screening assessment includes a narrow set of indicators of the environmental performances of the processes - excluding the assessment of the impact which mostly reflect the energy and material requirements for the production process. (See section 11.1.1).

A possible methodology combines simplified thermodynamic calculations, reaction process analogies, and "green chemistry" principles to estimate and compare the potential energy intensive unit operations of different chemical pathways and material designs. A summary of the methodology is described in Table 13.

Table 13. Possible methodology for the screening assessment of chemical/material.

Step	Description
1. Define System Boundaries and declared Unit.	The "production process" under evaluation should be delineated to include all relevant unit operations, such as one or more reaction steps, heating, mixing or separation operations, even in cases where only a basic reaction pathway has been proposed. To enable comparison between alternative process design options. Commonly, this may refer to a defined quantity of the target product—such as 1 kilogram or 1 mole—but should be selected based on the context of the assessment and the intended application of the results. The final application of the chemical may be undefined.
2. Break Down the Process into Unit Operations.	▪ Reaction: Including mixing, heating/cooling, pressure change operations. ▪ Separation/Purification: Distillation, filtration, crystallisation, extraction, drying and other unit operation needed to increase the concentration of a desired product or eliminate impurities and by-products. ▪ Solvent Management: Solvent use, recovery, and disposal. ▪ Ancillary Processes: Such as pumping, stirring, vacuum, inert atmosphere, utility generation.
3. Qualitative Hotspot Identification (here the example is based on the potential energy-intensive unit operations)	▪ High temperatures or pressures ▪ Multiple distillation steps ▪ Large solvent volumes ▪ Vacuum operations ▪ Recycling or purification of difficult-to-separate mixtures. ▪ Highly exothermic/endothermic reactions ▪ It is possible to use a qualitative score (e.g. low, medium, high) to prioritise data collection of the different unit processes.
4. Definition and calculation of indicators	▪ Reaction Enthalpy: This gives a first indication of heating/cooling demands. ▪ Theoretical Minimum Separation Energy: For ideal separations, it provides a fundamental lower bound and allows for comparison of separation difficulty. ▪ Boiling Points/Vapor Pressures: Large differences generally indicate easier distillation. ▪ Design principles of the framework
5. Evaluation and interpretation	▪ Identify key indicators (e.g. reaction temperature, solvent-to-product ratio, separation efficiency) that have a high impact on the result. these values can be compared with the ones provided in Table 14. ▪ Analyse the indicators change due to variation of process parameters to identify and prioritise R&D efforts.

Source: Own elaboration

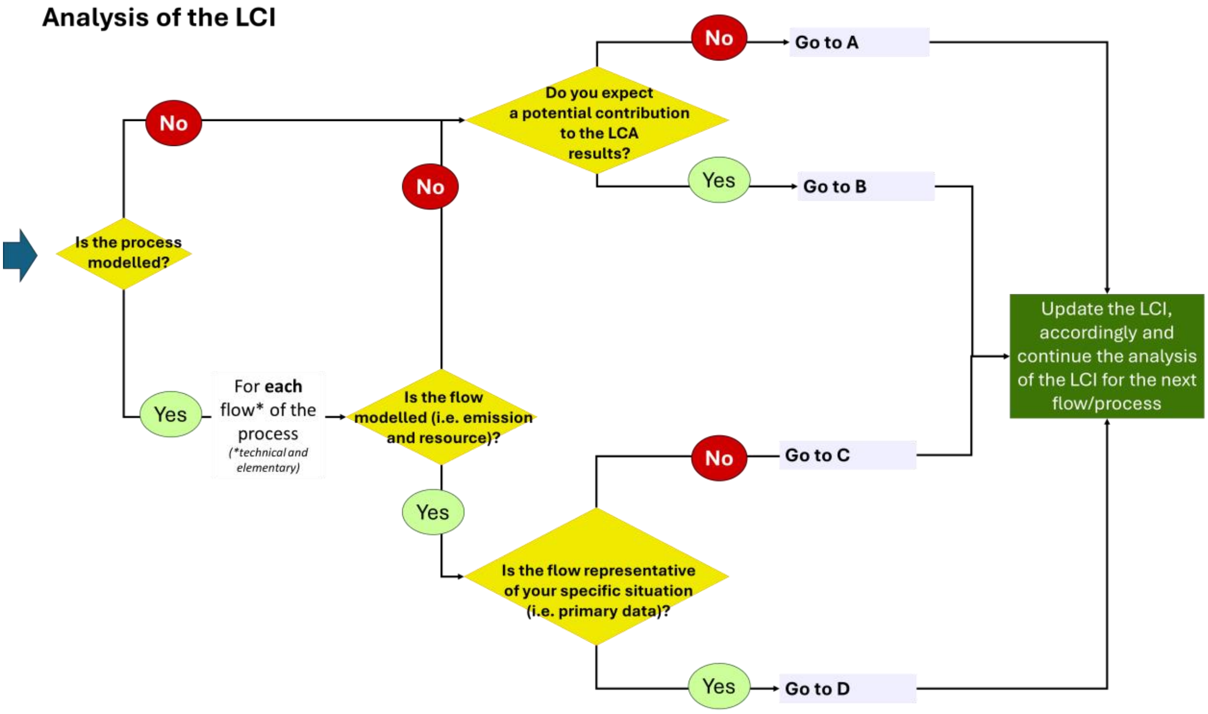
The **simplified, intermediate and full LCA** reflect the iterative and tiered approach of the implementation of the framework when the LCA is possible to undertake, even if only partially. Table 14 describes the main structure of the tiered LCA along the innovation, providing the main characteristics. Information on Goal and Scope definition, Life Cycle Inventory and Impact assessment are provided in the Methodological Guidance (Abbate et al., 2024), while here below information on the Results interpretation is provided.

The core of the evaluation of the environmental sustainability assessment is the interpretation of the LCA results, to understand how to proceed with the subsequent iteration. The evaluation should all look at the results from two different angles: the data quality for the Life Cycle Inventory (LCI) of the LCA model, and the identification of potential hotspots that should provide insights to the innovation. Figure 26 shows the two aspects of the evaluation with examples of questions and actions that aim at analysing the LCA model. Based on the information collected, the figure provides actions in both directions.

The analysis of the data quality to improve the LCI includes, among others, the analysis of the technological, geographical, time-related representativeness, completeness, uncertainty, and reliability of the data sources (further details are provided in Annex 7).

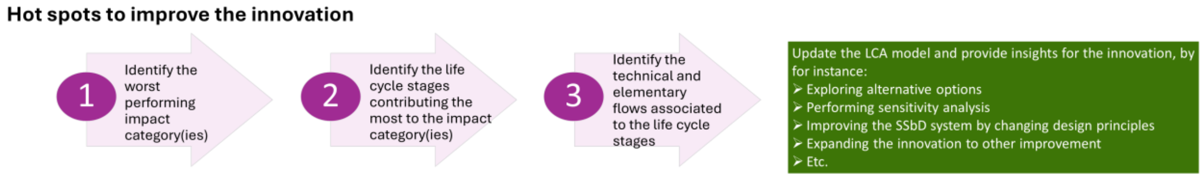
Figure 26. Possible approach to perform the interpretation of the LCA results, combining both the analysis of the data (a) and the obtained results (b).

(a)



A	Provide information on why the process and/or the omitted flows are not expected to contribute to the overall LCA results
B	1. List the omitted process and/or flows of the process 2. Analyse the potential contribution(s) of the omitted flows or process through various sources (e.g. literature review) 3. Collect information of the process and/or the omitted flows 4. Update the LCI with the collected information
C	**In this case the flow is *most likely* retrieved by database or literature**, the following actions may be considered: - Check the representativeness of the data (geographical, temporal, technological, etc.) - Collect a more representative information of the flow by improving the literature search or engaging with the suppliers/downstream users - Check the contribution of the flow to the overall process, and do a quick sensitivity analysis - Note that: in some cases, it is not possible to improve the representativeness of the flow – sensitivity analysis and uncertainty evaluation are suggested.
D	**In this case the flow is *most likely* retrieved by direct information (by the practitioner / suppliers or other actors along the life cycle)** , the following action may be considered: - Check the approach and assumptions to derive the flow - Check alternative values of the flow in literature - Perform some sensitivity analysis of the flow

(b)



Source: Own elaboration

Table 14. Summary of the main applicability and characteristics of the iterative and tiered approach of LCA along the innovation.

Tiered LCA	Simplified LCA	Intermediate LCA	Full LCA
Applicability	▪ Usually low maturity of innovation ▪ Data from laboratory most likely only from the innovator ▪ High uncertainty of the assessment ▪ Low/medium possibility to engage with the other actors of the value chain ▪ Un/Defined application(s)	▪ Increasing maturity of the innovation ▪ Data from industrial or pilot scale ▪ Medium/High uncertainty of the assessment ▪ Medium/high possibility to engage with the other actors of the value chain ▪ Defined application(s)	▪ High maturity of the innovation ▪ Data from industrial scale ▪ Low uncertainty of the assessment ▪ High possibility to engage with the actors of the value chain ▪ Defined application(s)
Indications on the life cycle (according to the levels of the (re)design selected)	▪ Molecular: the key life cycle stage is the synthesis/production of the chemical/material. Main life cycle to consider to be linked with the selected design principles, e.g. production and EoL. <u>Note: even if the use might unknown, consideration about the recyclability of the chemical/material is still possible</u> ▪ Process: the key life cycle stages are the production of the chemical/material, and the production of its precursors. The upstream process of the chemical/material can be prioritized in this phase ▪ Product: the key life cycle stages are the downstream stages, such as the product (containing the chemical/material) manufacturing, the use and the EoL	▪ Based on the level of the (re)design, prior effort shall be given in improving the life cycle stages more linked to the level of the (re)design – See below which improvements are iteratively needed in this phase ▪ The other life cycle stages shall be still considered with the needed assumptions and limitations already described in “Applicability”.	▪ The whole life cycle of the chemical/material shall be equally modelled and assessed with equal weight to conclude with the final evaluation, and so choice of the alternative – if applicable
Main characteristics	▪ A Simplified LCA helps to identify the most important life cycle stages and processes for data refinement, and thus guide the optimal use of effort and resources ▪ Knowing the product or sector application of the chemical/material under development, it is possible to create scenarios describing the possible variabilities, for instance in terms of geography or products. ▪ A very extreme initial phase to start the simplified LCA is to evaluate the indicators of the selected design principles	▪ This is the most iterative Tier of the LCA ▪ Continuous iterative adjustments of the simplified LCA modelling, which follows the increasing maturity of the innovation. ▪ Examples of refinement include primary data collection, filling in data gaps, inclusion of all the impact categories, and expanding the system boundaries to cradle-to-grave (as opposed to cradle-to-gate) ▪ Effort regarding the collection of primary data for LCI via in-house data collection, enhanced engagement with suppliers and/or downstream users, making specific data requests, etc.	▪ Final adjustments of the intermediate LCA ▪ The Full LCA includes adjustments that allows to follow the Recommendation of the European Commission to perform the LCA ▪ Adjustments mostly regard the refinement of the LCI, maximizing the engagement of the value chain ▪ Adjustments also regard the improvement of the modelling of the use and end-of-life phases

Source: Own elaboration

11.3. Process-related sustainability

As described in Chapter 6, the scoping analysis goes hand-in-hand with identifying what are the objectives of the SSbD with regard to the (re)design of a process. By assessing the chemical process(es)/technologies in their entirety, the SSbD can help to identify environmental pressures and potential impacts that might otherwise be missed[18].

At early stages of the innovation, LCA indicators may not be applicable to the processes under assessment and hence a preliminary sustainability assessment is needed. For this purpose, and integrating with the objective of the assessment of process related safety[19] (reported in section 10.4), the example below (Box 11) describes how some of the indicators listed in Table 11 can be used to identify possible hotspots in the industrial process from the environmental point of view.

In a later phase of the innovation, these indicators may be used to inform the LCA model to assess the process in a more complete fashion as it is described in section 11.2. Furthermore, when scaling up a technology toward its application at industrial scale, additional data and site-specific considerations might became available. In this case, also different indicators of environmental pressures could be chosen, and the assessment of the impacts could be refined, possibly aligning with environmental permitting schemes (for example the IED or the EIA).

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[18] For instance, a "green" synthesis method might be lauded for avoiding hazardous reagents in one step, but if it relies on energy-intensive purification techniques or generates large volumes of difficult-to-treat waste downstream, and this its overall “whole life” environmental benefit is diminished. Similarly, a process might seem efficient, but if it uses highly toxic or non-renewable raw materials, or if its byproducts pose long-term environmental hazards, the perceived performance is misleading.

[19] Efforts to promote environmental sustainability in the industrial and chemical sectors have predominantly focused on Life Cycle metrics evaluating impacts along the supply chain. While these indicators are essential for assessing environmental performances, they may not sufficiently capture other dimensions of sustainability, particularly those related to human health and environmental safety arising from the processes involved in the value chain, where site specific conditions need to be considered

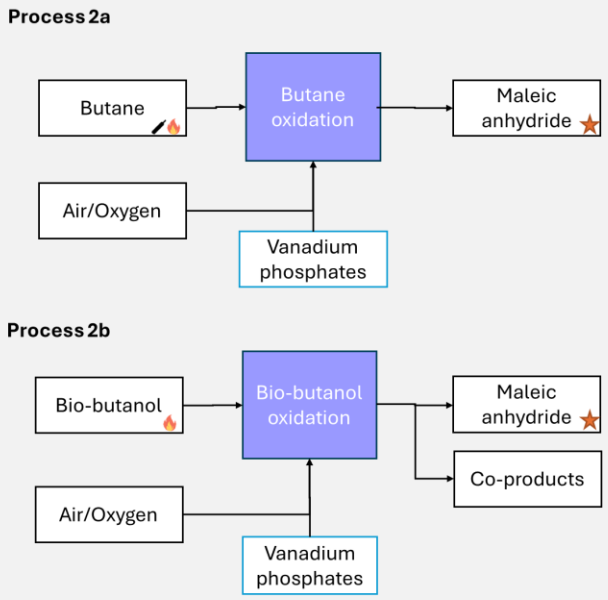
Box 11. Screening of process-related sustainability at early stage of process development.

Continuing the example reported in **Box 10**, the environmental sustainability of the maleic anhydride synthesis processes is explored. A selected number of indicators are used to compare the two processes on crucial aspects: namely, the quantity and type of raw materials, the presence of stoichiometric CO_2 emissions and the heat of reaction. These indicators are used to highlight preliminary hotspots that may emerge already at theorical level, before process design starts.

The chosen indicators are selected since they are linked to main drivers of environmental impacts, such as emission of direct fossil CO_2 and energy consumption. Moreover, they are based on intrinsic properties of the chemicals and the reaction (e.g. heat of formation and stoichiometry) and are therefore appropriate to the early stage of assessment.

After a preliminary screening of process 1 and 2 using these indicators, it can be noted that process 1 has one major hotspot due to the fossil feedstock and CO_2 production in the reaction. On the other hand, process 2 still has a major drawback of relying on a fossil feedstock. For this purpose, the practitioner may investigate alternative sources of butane, or similar synthesis routes which allow for the use of existing renewable feedstocks. For example, the partial oxidation reaction can be done also starting from butanol (Cucciniello et al. 2023), which is available from biomass fermentation. Hence, a variant of process 2 can be added to the screening both for the environmental and the safety aspects.

At the first level of the screening, process 2b misses all the selected sources concern compared to process 1 and 2. Also from the process safety perspective, using butanol as feedstock eliminate the risks associated to pressurized gases. In the next iteration of development, when preliminary calculation on process design will be performed, other indicators should be selected to account for more parameters, such as reaction yield (which depends on the reactor type and design) or separation efficiency.



	Process 1	Process 2a	Process 2b
Fossil feedstock	X	X	
CO_2 emissions	X		
Reaction yield	High	Low	Low
E-factor	1.26	0.735	0.734
Energy of reaction	Exoth.	Exoth.	Exoth.

Source: Own elaboration

12. Socio-economic sustainability assessment

12.1. Rationale and objectives

Within SSbD, the socio-economic sustainability assessment aims at complementing the safety and environmental sustainability assessments with the identification and, where possible, quantification of socio-economic risks and opportunities in the innovation process. In line with the current EU policy priorities and with the aim of contributing to the Sustainable Development Goals (UN General Assembly, 2015), its goal is to help identify the relevant tools and indicators that can help the SSbD practitioner to:

- Promote social fairness and minimise the risk of human rights abuses and poor working conditions in the value chains
- Promote innovation and competitiveness through more resilient and sustainable value chains
- Support risk management and mitigation along the life cycle (including ethical and reputational risk, risk of supply chain disruption and financial risks due to accidents and hazardous processes), facilitating information sharing and transparency along the value chain and raising awareness in B2B and B2C communication
- Identify opportunities and socio-economic benefits as well as costs and externalities of different choices within the innovation strategies.

In line with the objectives stated above, the socio-economic analysis is composed of two main pillars:

1. **Social fairness:** the socio-economic analysis should strive to steer innovation towards producing societal benefits, while ensuring equal opportunities, health and safety, fair working conditions and respect of human rights.
2. **Competitiveness**: the socio-economic analysis should ensure that supply chain vulnerabilities are considered, improving preparedness and risk management and ensuring economic and financial security.

The socio-economic assessment is designed to **complement and build upon** the analyses conducted in the previous steps of the SSbD assessment. While earlier steps may already consider specific social concerns (e.g. hazardous properties and exposure risks associated with a substance or material), the socio-economic assessment provides a **systematic and structured evaluation** of the broader socio-economic dimension along the life cycle of a chemical or material, including human rights, health and safety, working conditions and competitiveness. In the longer term, this step could facilitate and support the integration of sustainability and risk-related criteria into investment decision making.

This step is closely linked to previous steps through shared methodological foundations—particularly the use of Life Cycle Assessment (LCA) for defining system boundaries and functional units. These elements ensure coherence across the environmental and socio-economic assessments.

Moreover, the socio-economic assessment builds on the scoping exercise and environmental Life Cycle Inventory already performed, streamlining the integration of socio-economic indicators by using the same SSbD system definition.

The influence of the initial scoping analysis is particularly critical in shaping the socio-economic assessment, as it defines not only the system boundaries but also the scope and granularity of the data considered. Decisions made during this early phase of innovation and design (e.g. commitments to source only certified, ethical, and sustainable raw materials) play a foundational role in determining which socio-economic impacts are included and how they are assessed. These assumptions and commitments should be transparently documented to allow for traceability and consistency across iterations of the assessment.

12.2. Aspects, indicators and criteria definition

Considering the pillars underpinning the socio-economic analysis, a list of proposed socio-economic aspects and categories to prioritise in the context of the SSbD is presented in Table 15. These categories have a varying dependency on the technology features, which has been indicated in the table following the taxonomy developed in Hannouf et al. (2025). Having awareness of this feature is important when establishing the relationship between the chemical/material under investigation and social impacts. Indeed, social inventory data can be collected at different scales: product, company, and sector/country level.

Table 15. List of pillars, socio-economic aspects and categories that may be included in the socio-economic assessment.

Pillar	Socio-economic aspect	Socio-economic category	Dependence on technology feature (based on Hannouf et al. 2025)
Social Fairness	Human rights	Risk of child labour in the supply chain	c
		Risk of forced labour in the supply chain	c
	Working conditions and quality of jobs	Fair salary	c
		Working time	c
		Equal opportunity and discrimination	b
		Freedom of association and collective bargaining	c
	Health and safety	Accidents at work	a
		Presence of safety measures	a
		Safe and healthy living conditions	a
Competitiveness	Contribution to economic development	Contribution to economic development	a
		Creation of knowledge-intensive employment	a
	Supply chain vulnerabilities	Risk of supply disruptions	a
	Skills and technology innovation potential	Technology potential	a
		Skill shortages risk	a
Societal Life Cycle Costs	/	/	a

Source: Own elaboration (a: aspects relevant to technology features; b: with relevance that depends on the technology type; c: independent of technology feature; adapted from Hannouf et al. 2025)

The selection of these socio-economic aspects was based on the previous SSbD work conducted by the JRC, including the 2022 SSbD review (Caldeira et al., 2022a) and framework (Caldeira et al., 2022b), the case study application (Caldeira et al., 2023) and the Methodological Guidance (Abbate et al., 2024). Moreover, additional literature sources related to socio-economic assessment of emerging technologies was consulted (Grimaldi et al., 2020; Padilla-Rivera et al., 2023; Pérez-López et al., 2025; Popien et al., 2025; Sell et al., 2014; Díez-Hernández et al. 2026; Stoycheva et al. 2022; Pucciarelli et al. 2020; Cadena et al. 2019; Hannouf et al. 2025; Rafiaani et al., 2020; van Haaster et al., 2017). The selection also considered the availability of open-source databases, to facilitate the application of the socio-economic analysis to a wide group of practitioners.

The assessment of the socio-economic aspects listed above should be based on three distinct complementary steps:

1. Assessment of social risks and opportunities along the value chains using a **Reference Scale Assessment** (ISO 14075, 2024.): this approach is used in Social Life Cycle Assessment (S-LCA) to assess potential socio-economic impacts and builds on the modelling performed in the environmental LCA. In particular, the same functional unit (i.e. the function/service provided by the chemical/material) defined in the LCA can be used in this analysis, while the system boundaries should be adapted and simplified to consider only the phases of the value chain that are relevant from the socio-economic point of view. In the context of the SSbD, however, a simplified methodological approach is suggested, especially at low levels of innovation maturity and in this case the use of a functional unit is optional.
2. **Identification of Critical Raw Materials (CRM)** along the life cycle: this phase implies the use of Life Cycle inventories developed in LCA and the flagging of the CRMs used as inputs in the production processes, including the upstream phases of the value chain (i.e., including intermediate products and raw materials used as precursors).
3. **Assessment of life cycle costs, including societal costs**[20]: where a comparison between different alternatives is to be made, this analysis allows the identification of the cost-optimal option over the lifetime of a chemical/material, including the consideration of externalities. The use of the simplified EcoReport tool used in the context of Eco-design (Gama Caldas et al., 2024) can facilitate the assessment.

Concerning the third point on life cycle costs, the role of the socio-economic assessment in SSbD is not to duplicate corporate financial analysis, but rather to support and complement the assessment of internal costs with additional economic considerations on externalities (e.g. societal costs) and financial risk related to hazardous or poorly sustainable processes. A focus on the latter aspects is presented in section 12.4. An overview of current methods and data estimating externalities, together with the related levels of uncertainty, is provided in (Amadei et al., 2021).

In this sense, the SSbD socio-economic assessment complements profitability analysis by helping innovators and companies to consider the socio-economic risks and opportunities of their designs —

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[20] In this context, and in accordance with the EcoReport tool used in the context of Eco-design (Gama Caldas et al., 2024), **societal costs** refer to the monetised results of the LCA impact categories, using the monetisation factors provided in Annex 7.

including potential risks, costs, and benefits that extend beyond the firm level. In addition, the framework aims to steer innovation towards strengthening EU competitiveness by assessing aspects such as technology potential, skills development, and the creation of knowledge-intensive employment. In doing so, it helps companies not only comply with safety and sustainability principles but also position themselves strategically in evolving markets and policy landscapes.

Assessment methods and indicators

Table 16 provides information on the set of assessment methods and indicators that may be used for the assessment of each socio-economic aspect.

The assessment uses both primary data (i.e. quantitative or qualitative values obtained by direct measurement, or a calculation based on a direct measurement or observations at original sources) and secondary data from literature and databases.

Table 16. Set of proposed categories, aspects, methods, and indicators.

Impact category	Socio-economic aspect	Assessment method	Examples of indicators	Source
Human rights	Risk of child labour in the supply chain	Reference scale assessment	Proportion of children engaged in economic activity (%)	SDG Labour Market Indicators (ILOSDG)
	Risk of forced labour in the supply chain	Reference scale assessment	Global Slavery Index Goods produced by forced labour	Walk Free Foundation US Department of Labor
Working conditions and quality of jobs	Fair salary	Reference scale assessment	Average monthly earnings of employees by sex and economic activity	ILOSTAT Wages and Working Time Statistics (COND)
	Working time	Reference scale assessment	Mean weekly hours actually worked per employed person by sex and economic activity	ILOSTAT Wages and Working Time Statistics (COND)
	Equal opportunity and discrimination	Reference scale assessment	Gender wage gap (%) Proportion of women in senior and middle management positions (%)	SDG Labour Market Indicators (ILOSDG)
	Freedom of association and collective bargaining	Reference scale assessment	Level of national compliance with labour rights (freedom of association and collective bargaining)	SDG Labour Market Indicators (ILOSDG)
Health and safety	Presence of safety measures	Reference scale assessment	Preventive measures and emergency protocols exist regarding: i) accidents and injuries, ii) pesticide and chemical exposure Adequate general occupational safety measures	UNEP 2021 (Methodological Sheets for Subcategories in S-LCA 2021)
	Accidents at work	Reference scale assessment	Fatal/non-fatal occupational injuries per 100'000 workers	SDG Labour Market Indicators (ILOSDG)
	Safe and healthy living conditions	Reference scale assessment	Organisation efforts to strengthen community health (e.g. through shared community access to organisation health resources) Management effort to minimize use of hazardous substances and control of structural integrity	UNEP 2021 (Methodological Sheets for Subcategories in S-LCA 2021)
Contribution to economic development	Contribution economic development	Reference scale assessment	Contribution of the product/service/organisation to economic progress (e.g. annual growth rate of real GDP per employed person)	UNEP 2021 (Methodological Sheets for Subcategories in S-LCA 2021)
	Creation of knowledge-intensive employment	Reference scale assessment	Average proportion of skilled workers, out of all workers (%) Knowledge intensive jobs (% high-skilled employees (ISCO level 3-4) /total employees required for a unit of production)	World Bank Enterprise Survey
Supply chain vulnerabilities	Supply chain vulnerabilities	Identification of CRM	N° of flags related to the presence of CRM as material inputs, based on EC methodology. Mass of CRMs/total material input; additional qualitative assessment of supply chain vulnerability.	EU Study on the Critical Raw Materials for the EU 2023 (European Commission 2023)

Impact category	Socio-economic aspect	Assessment method	Examples of indicators	Source
Skills and technology innovation potential	Technology potential	Reference scale assessment	Involvement in technology transfer program Projects partnerships in research and development Investments in technology development/ technology transfer Patent growth rate in % of this technology for a defined period (e.g. 5 years).	UNEP 2021 (Methodological Sheets for Subcategories in S-LCA 2021)
	Skill shortages risk	Reference scale assessment	Ratio of training investment per employee vs. industry benchmarks. Qualitative assessment about the extent to which the company contributes to skill development for the community at large.	ORIENTING. (2023). (D2.5) Specification of social indicators for LCSA. EU Horizon 2020 project ORIENTING (GA No 958231)
Societal Life Cycle Costs	/	/	Internal costs (incl. e.g. material acquisition, labour, energy, etc) Externalities (through monetisation of LCA impacts)	Gama Caldas, et al. (2024) Review of the MEErP - Methodology for Ecodesign of Energy-related Products.

Source: Own elaboration

It should be noted that the assessment of **supply chain vulnerabilities** within the SSbD framework currently includes the identification and flagging of Critical Raw Materials (CRMs) along the life cycle, reflecting concerns around strategic dependencies and geopolitical risks. However, to provide a more **comprehensive understanding of supply chain resilience,** this aspect should not be limited to CRM-related risks alone. Other factors such as energy supply disruptions, water scarcity, and the general availability of essential raw materials (e.g. bio-based feedstocks, chemical molecules, catalysts for reactions) can significantly affect the sustainability and security of value chains. These broader dimensions of vulnerability are particularly relevant in the context of climate change, shifting global trade dynamics, and resource competition.

While the current framework lays the foundation by flagging CRM risks, the analysis of supply chain vulnerabilities can be complemented with qualitative information on other potential factors of risks, e.g.:

- trade risks due to tariffs and trade barriers
- knowledge and skills shortages
- exposure to energy price volatility
- vulnerability to climate change and extreme weather events
- armed conflicts

The methodological guidance will address these additional factors in more depth, supporting more systematic risk screening.

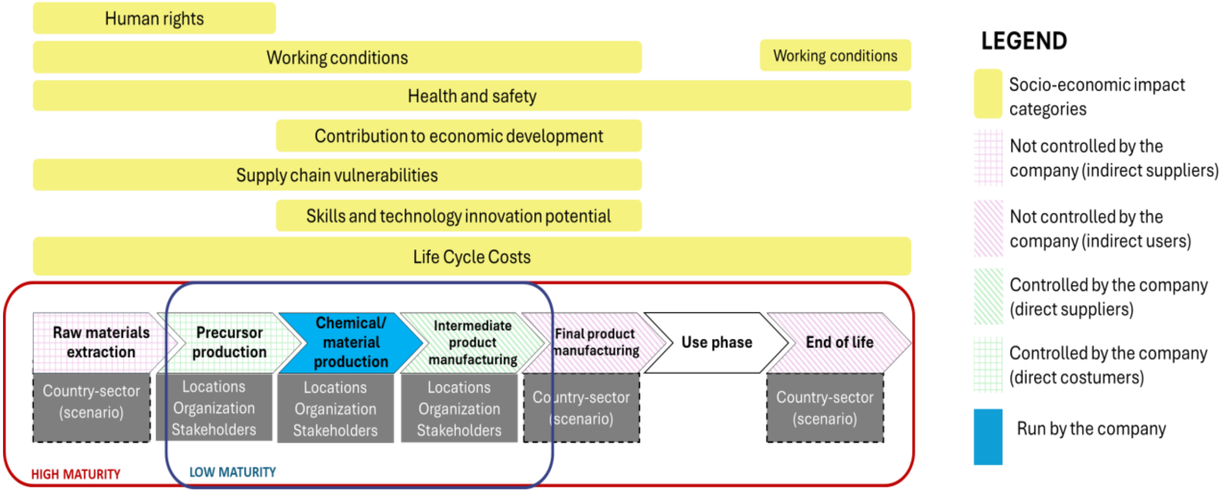
The indicators shown in Table 16 can be calculated at different levels and using data with different granularity:

- **Chemical/material level:** usually it is not possible to have this level of detail for social data, or simply the type of chemical and material is not relevant for the specific socio-economic aspect. However, the type of chemical and material has an influence when modelling the system boundaries, as the entire value chain should be represented in terms of involved country-sectors. Instead, data on costs can be specific for the chemical and material under investigation, even though at low innovation maturity levels these can be difficult to estimate.
- **Corporate level:** data at corporate level may be used to assess the social responsibility of business partners downstream and upstream in the supply chain. Primary data can be obtained through interaction with stakeholders or indirectly from sustainability reports and other sources.
- **Country-sector level:** data on the sector is usually available from statistics and databases and allow to assess the parts of the value chain that are more remote and for which primary data collection is not possible. In some cases, these data are available only at country level and can be used to obtain an estimate of the potential risk in global value chains.

The use of primary data enhances the robustness of the assessment; however, secondary data can also be used to perform simulations of potential value chains with limited costs and effort and are useful when potential business partners are still unknown.

The level of maturity of the innovation greatly influences the application of the socio-economic analysis. As shown in Figure 27, at low innovation maturity levels the analysis can be limited to the operation of the company itself which is performing the assessment, and direct business partners, while the boundaries may be extended at increasing innovation maturity levels.

Figure 27. Level of application of each impact category considering the life cycle of a chemical/materials and the maturity of the innovation.



Source: Own elaboration

A robust methodology for the socio-economic assessment should include clear, actionable criteria that enable the benchmarking of sustainability performance. For the three steps proposed for the analysis the following strategies can be followed:

1. Development of criteria for social aspects

Social Life Cycle Assessment (S-LCA) provides a foundation for evaluating social risks and benefits across the life cycle of a product or process. Reference scales, often used in S-LCA, enable the classification of performance across a continuum—from very low to very high risk/benefit—based on predefined benchmarks such as international norms (e.g. ILO standards, International Conventions, etc.). In the context of SSbD, the reference scales can serve as exclusion or prioritisation criteria, specifically:

- **Criterion definition**: Processes or supply chain phases that fall within the "high" or "very high" risk categories on the reference scale for key social aspects (e.g. forced labour, child labour, unsafe working conditions, community displacement) can be flagged as non-sustainable.
- **Operationalisation**: A threshold-based cut-off can be applied where options exhibiting high/very high risks are either excluded from further consideration or require mitigation strategies.

This step integrates ethical boundaries into the design process, steering innovation away from socially harmful practices.

2. Identification and Flagging of Critical Raw Materials (CRMs)

The use of Critical Raw Materials —defined by the European Commission in its list, periodically revised — is essential for many strategic technologies and can provide technological functions that are hardly replaceable. Their use in the chemical/material supply chain, while not negative per se, should be monitored in order to increase awareness on potential supply chain bottlenecks due to supply insecurity and geopolitical dependencies.

Criteria for this component of the evaluation are twofold:

- **Flagging criterion**: the presence of CRMs in the life cycle (i.e. input flows in the life cycle inventories). The number of flags (i.e., unique CRMs used) and the total mass of CRMs can be used as quantitative indicators.
- **Comparative and design-based evaluation**: these metrics (number of flags and total mass of CRMs) support the comparative evaluation of alternatives and encourage innovation toward CRM substitution or minimisation, aligning with SSbD design principles. While a single flag does not automatically disqualify a design option, multiple flags or a high CRM mass content may indicate a lower sustainability profile.

Thus, the criteria for this part serve not as an absolute cut-off, but rather as a driver for continuous improvement and material innovation.

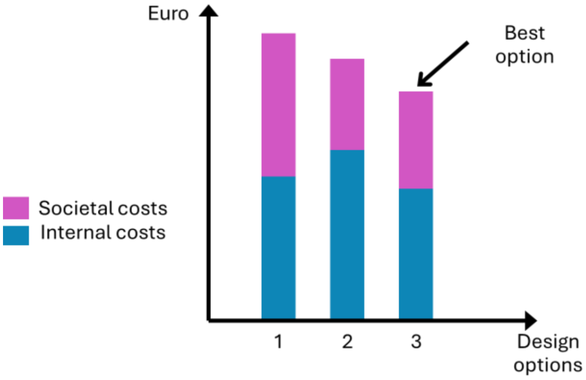
3. Life Cycle Costs

Criteria in this dimension are framed in comparative terms only and can allow the inclusion of externalities in the consideration of alternative design options, as displayed in Figure 28.

- **Comparative criterion**: The sustainability of a chemical or material is assessed relative to alternatives based on total cost across the life cycle, including societal costs (including, for instance, damage costs due to environmental and health impacts, or the energy gains for the consumer due to a more energy efficient product). The preferred option is that which entails the lowest total cost (i.e. including both internal and societal costs), whilst maintaining an equal level of technical and functional performance.
- **Benchmarking role**: While absolute thresholds are difficult to define, comparative Societal Life Cycle Cost (S-LCC) allows for ranking of options and identification of trade-offs, which can be fed back into the design loop for optimisation.

In this way, S-LCC criteria promote cost-effective sustainability by internalising negative externalities and revealing the true socio-economic footprint of design choices. The overall methodology takes its inspiration from the Method for the Ecodesign of Energy-related Products (MEErP) (Gama Caldas et al., 2024), but in an adapted version, taking into account inputs from primary LCA and cost data collected by the innovating entity, supplemented by background data from LCA and financial / utilities databases (where the maturity of the innovation of the system under analysis is sufficiently high to allow this level of assessment).

Figure 28. Comparison of Life Cycle Costs of different design options.



Source: Own elaboration

12.2.1.Development of reference scales and scoring system

Building on the methodological foundations of Social Life Cycle Assessment (S-LCA), the development of reference scales and a scoring system allows for consistent benchmarking and prioritisation of social performance across alternative design options. This chapter presents how reference scales can be developed based on measurable indicators, and how they can be translated into a scoring framework to support SSbD decision-making. The reference scales and the scoring are applicable for the aspects under the assessment steps 1) social risks and opportunities via Social LCA and 2) identification of CRM, but it should be noted that they do not apply to step 3), i.e., the inclusion of life cycle costs considerations.

Reference scales provide a structured way to classify the social performance of an SSbD system, a company or supply chain stage against internationally recognised norms and best practices. These scales are typically ordinal (e.g. from "very high risk" to “very low risk” and from “worst practice” to "best practice") and are built around quantitative and qualitative indicators.

For several indicators related to social risk at country-sector level, reference scales are available in (Loubert & Maister, 2023) and an example is reported below. Reference scales for all the indicators are proposed in Annex 8, noting that these are not fixed values; reference scales can also be built based on existing standards and sector-specific benchmarks. However, the reasoning and sources for the definition of reference scales should be transparently documented.

Once reference scales are defined, a scoring system allows the translation of performance levels into numerical values, enabling aggregation across multiple indicators and social aspects. An example of scoring for the indicator of “% of children in employment” is presented in Figure 29.

Figure 29. Example of reference scale set for the social indicator “% of children in employment”.

Indicator value y, % of children in employment aged 5-17	Risk levels	Assigned score
0 < y < 2.5	Very low risk	4
2.5 ≤ y < 5	Low risk	3
5 ≤ y < 10	Medium risk	2
10 ≤ y < 20	High risk	1
20 ≤ y	Very high risk	0

Source: Loubert & Maister, 2023

In the case of socio-economic aspects that are assessed at corporate level and with qualitative data, the reference scale can be designed taking into account the performance of the company compared to best practice. An example for the socio-economic aspects “Skill shortages risk” is shown in Table 17.

Table 17. Example of reference scale for the assessment of “skill shortages risk” with company level qualitative data.

Definition	Performance level and assigned score
The company actively invests in reducing the skills mismatch in the region and invests in a public private partnership or invests in other activities that significantly increase training capacity and quality in the region for most members of the local community, not specifically guided by the company’s own needs.	4
The company actively contributes to reducing the skills mismatch, by offering skill development for a relevant share of members of the local community.	3
The company is managing the skill gap in a way that members of the local community are sufficiently qualified when new staff are hired.	2
There is a significant skill-gap between the future needs of the company and the skill levels of local community members, but the company has started to address this with an action plan with a clear timeline.	1
There is a significant skill-gap between the future needs of the company and the skill levels of local community members. The company is planning to perform some actions to improve this situation in the future.	0

Source: Own elaboration, adapted from (Zanchi et al., 2024.)

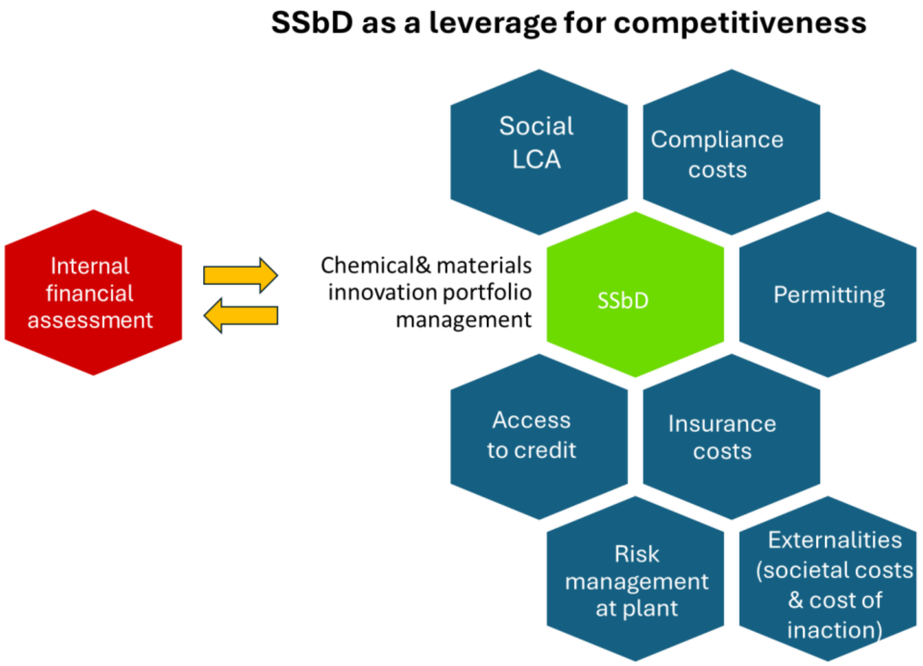
12.3. SSbD as a strategic lever for competitiveness and financial resilience

SSbD could act as strategic driver of innovation, enabling long-term competitiveness for companies operating in chemicals, materials, and manufacturing sectors. By embedding safety, sustainability, and risk minimisation into the earliest stages of design, SSbD can help organisations make more informed investment decisions, manage financial exposure, and access new funding opportunities.

At the core of this dynamic lies the interplay between technical design, risk governance, and financial performance. SSbD provides a framework for aligning product development with emerging ESG (Environmental, Social, Governance) expectations.

As shown in Figure 30, the adoption of SSbD could be a leverage of competitiveness in many ways. By proactively addressing regulatory, financial, and reputational risks companies can avoid costly redesigns or market restrictions whilst at the same time gaining a first-mover advantage. The SSbD could also contribute to improved insurability, as safer designs and strong sustainability performance could lead to lower premiums and better coverage in the insurance market. Financial institutions increasingly favour ESG-aligned companies, and SSbD-aligned operations could benefit from sustainability-linked loans or lower interest rates due to their reduced risk profiles.

Figure 30. Role of SSbD vis a vis elements of competitiveness



Source: Own elaboration

While these competitiveness-related aspects cannot be exhaustively assessed in a quantitative manner in the current SSbD framework, their consideration and integration in the decision-making process can positively contribute to risk mitigation and preparedness.

The cumulative effect of these factors creates a self-reinforcing beneficial cycle: lower inherent risks improve insurability and creditworthiness, facilitating possible access to more favourable financial terms and capital for reinvestment in innovation. Conversely, companies that fail to address risks may face higher insurance costs, financing barriers, and reputational damage, this potentially limiting their long-term competitiveness.

12.4. Data sources, uncertainty and limitations

A variety of publicly available and proprietary databases can support the quantification and classification of social aspects, both at the country and sector level. Below there is an overview of relevant sources per indicator group (Table 18). The following sources are useful mainly for data at country-sector level, while the collection of primary data should be based on the collaboration of stakeholders and business partners in the assessment. In addition, information at company level for some indicators (e.g. gender gap, accidents at work) can be retrieved from sustainability reports.

Table 18. List of potential data sources.

Social Aspect	Main Data Sources
Child labour	UNICEF (United Nations Children's Fund), ILOSTAT (International Labour Statistics), World Bank World Development Indicators, Product Social Impact Life Cycle Assessment (PSILCA); Social Hotspot Database (SHDB)
Forced labour	Walk Free Foundation, US Department of Labor, ILO Global Estimates of Modern Slavery, PSILCA, SHDB
Fair salary	WageIndicator Foundation, ILOSTAT, World Bank
Working time	ILOSTAT, Eurostat Labour Force Survey, national statistical offices
Occupational safety	ILOSTAT, Eurostat, national ministries of labour/safety
Equal opportunity (gender gap)	ILOSTAT, OECD Gender Data Portal, World Economic Forum Gender Gap Report
Freedom of association & collective rights	ITUC (International Trade Union Confederation) Global Rights Index, ILO NATLEX, PSILCA, SHDB
Contribution to GDP	World Bank, UNDP, OECD.Stat, national accounts
Knowledge-intensive employment	World Bank Enterprise Survey, Eurostat, OECD (Labour Force by Skill Level), national labour force statistics
Supply chain vulnerability	IEA Energy Statistics; Global Conflict Risk Index; World Economic Forum The Global Risks Report
Technology potential (patent growth)	World Intellectual Property Organisation, European Patent Office Observatory on Patents and Technology, USPTO (United States Patent and Trademark Office) databases; OECD Patent Statistics

Source: Own elaboration

Social data used in sustainability assessments are often **incomplete, unevenly distributed**, and **context-dependent**, which introduces uncertainty into both classification and scoring. To address this, the evaluation of **data quality** is essential and should consider several dimensions:

- Reliability of data sources
- Completeness conformance
- Temporal conformance
- Geographical conformance
- Further technical conformance

A practical approach for managing uncertainty is the **pedigree** matrix (see Annex 8), which can assign scores to each dimension of data quality, helping to track and communicate uncertainty levels. Alternatively, semi-quantitative uncertainty ratings (e.g. low/medium/high uncertainty) can be attached to each score or indicator (More details in Annex 7Annex 7).

While the integration of the socio-economic analysis into SSbD provides valuable insights, especially in terms of raising awareness of potential ethical risks in the value chain, some limitations should be acknowledged:

- **Data availability and granularity**: Many indicators are available only at national or sector level, limiting site-specific relevance. Moreover, the complex nature of value chains and the variety of suppliers that the company deals with increases the complexity of the assessment.
- **Trade-offs and aggregation**: Aggregating scores across indicators risks masking critical issues (e.g. a good score on wages offsetting a high child labour risk).
- **Static nature of risk data**: social risks can evolve rapidly (e.g. due to conflict, policy change), whereas data may reflect past conditions.
- **Limited causality**: most indicators describe conditions or risks, not actual impacts attributable to a specific chemical or materials.
- **Feasibility of robust socio-economic assessment at low maturity of innovation:** the production system, supply chain, or life cycle configuration may still be undefined or hypothetical at low innovation maturity levels. This constrains the socio-economic assessment especially for site- or actor-specific indicators (e.g. wages, employment creation, accidents).
- **Uncertainty of cost estimates at low maturity of innovation**: Cost data for emerging materials or technologies are often incomplete, speculative, or based on laboratory-scale results. This limits the reliability of **life cycle costing (LCC)** or traditional cost-benefit analyses. Key assumptions (e.g. scale-up factors, process yields, energy intensity) may vary significantly, introducing large uncertainties that are difficult to quantify consistently across alternatives.
- **Challenges in tracing Critical Raw Materials (CRMs):** early-stage designs may not have fully specified bills of materials or supply chain configurations, making it difficult to accurately estimate CRM content or sourcing risks**.**
- **Uncertainties in the monetisation factors for the externalities**: There are several approaches to calculate monetary valuation coefficients. A number of coefficients has already been proposed in Commission initiatives (Gama Caldas et al., 2024), and are proposed in the context of SSbD. However, for some environmental impact categories, the level of uncertainty is too high to allow for a robust estimate, and monetisation values are lacking.

These limitations suggest the need for **iterative use** of the assessment, supporting early decision-making but also recognising when deeper engagement (e.g. stakeholder consultation, supplier audits) is necessary. Moreover, socio-economic analysis is more suitable for comparative and relative evaluations (rather than absolute assessments). Finally, document assumptions, data gaps, and sources of uncertainty should be transparently documented (Chapter 14).

12.5. Synergies with other socio-economic analyses

The socio-economic analysis developed within the SSbD framework presents some potential for alignment and synergy with key regulatory and corporate instruments in the EU policy landscape. Notably, it links and complement the Socio-Economic Analysis (SEA) under the REACH Regulation, the reporting requirements introduced by the Corporate Sustainability Reporting Directive (CSRD)

(EC, 2024c), and the due diligence obligations established by the Corporate Sustainability Due Diligence Directive (EC, 2024d).

In this context, synergies can be identified with these other forms of socio-economic analyses, given that some tasks performed by companies or data collected for other purposes can also be used for the socio-economic assessment of the SSbD. Table 19 summarises the main common elements between the SSbD and the most relevant related socio-economic assessment performed under the EU legislation.

Table 19. Envisaged synergies between the socio-economic assessment in SSbD and other socio-economic analyses.

Policy/document	Level of the analysis	Aim	Envisaged synergies with socio-economic assessment in SSbD
Corporate Sustainability Reporting Directive (CSRD) (EC, 2022b)	Corporate	Establishes rules concerning the social and environmental information that companies have to report, through the European Sustainability Reporting Standards (ESRS)	Assessment of performance through the Reference Scale Approach
Directive on corporate sustainability due diligence (Directive 2024/1760) (EC, 2024c)	Corporate	Requires companies operating within the European Union to conduct due diligence throughout their supply chains to identify, prevent, mitigate, and account for adverse impacts on human rights, the environment, and governance issues.	Modelling of the supply chain Identification of social risks Engagement with business relationships in the value chain
Socio-Economic Analysis within the ECHA authorisation process under REACH regulation (ECHA, 2011)	Substance	Assess the socio-economic impacts of the continued use of a substance subject to authorisation, or in the assessment of alternatives	Identification of social impacts Data collection on e.g. working conditions Definition of scenarios for application/use of the chemical/material Life Cycle Costing

Source: Own elaboration

13. Evaluation

The aim of the evaluation is to support the decision-making process along the innovation cycle of chemicals/materials within the frame defined by the scoping. To this end, this chapter includes:

- An overview of potential strategies to navigate trade-offs among the dimensions considered in the framework, including safety and environmental, social and economic sustainability.
- An example of how the outcome of a scoping analysis and the results of the safety and sustainability assessment may be visualised, considering the maturity of the innovation and the degree of uncertainty.
- An example of how the results of the safety and sustainability assessment, and possibly other aspects, might be evaluated using Multi Criteria Decision Analysis (MCDA).

The evaluation compares the outcomes of the assessment of safety and sustainability aspects, which should be based on the criteria described from chapter 10 to chapter 12, with the objectives and decision-making rules for safety and sustainability dimensions and the overall SSbD implementation in innovation.

Possible outcomes of the evaluation, depending on the iteration, can be:

- Additional information is needed / uncertainty should be reduced.
- Objectives should be refined.
- (Re)design should be refined.
- All possible refinements have been applied after a number of SSbD iterations and a sufficient degree of certainty regarding the safety and sustainability assessment has been achieved.

13.1. Trade-offs and decision-making in the SSbD framework

Trade-offs can be generally defined as situations characterised by conflicts among the desired objectives, where it is impossible to satisfy all criteria simultaneously (Kravchenko et al., 2020).

While the SSbD framework allows for the visualisation and possibly for the solving of the trade-offs within and between the different aspects of the safety and sustainability dimensions, it is acknowledged that in innovation process the trade-off considerations go beyond these, and other aspects need to be considered, such as the functionality and the market considerations (e.g. penetration, consumer price, etc.) .

The decision making is a continuous process that takes place throughout the entire innovation. The use of decision-making rules is one important approach to formalise and to make the decisions that occurred during the innovation more systematic and explicit.

Decision-making rules can be defined early in the scoping analysis to screen out alternatives, and they can be used to guide the quality of data, and how data gaps will be considered. Sometimes, decision-making rules are inherent in the choice of method or tool used to support the assessment.

Additional decision rules come into play in the final decision-making stage of the assessment where trade-offs are likely to occur (Malloy et al., 2017). Additional decision rules might need to be considered to address potential trade-offs in the final decision-making. It should be also noted that decision-making rules may change along the innovation process (where other aspects, in addition to safety and the sustainability dimension are considered, such as the technical performance or the technical/economic feasibility). When implementing the SSbD framework, trade-offs in the safety and environmental performance should be limited as much as possible (e.g. by considering the minimum requirements for each dimension), so that **one aspect cannot overrule unacceptable weaknesses on the others** (Dias et al., 2024).

Different methodologies exist for navigating trade-offs and making decisions. Table 20 provides an overview of some methodologies (OECD, 2021), that have been adapted for SSbD. Some of these strategies are relatively simple to implement, such as eliminating “high ratings”, while others require more sophisticated assessments, such as “weighted scoring of endpoints”.

The best approach will be the use of case specific factors, such as the resources available, chosen by the SSbD practitioner. Nevertheless, engagement with the life cycle actors and documentation of the strategy remains key.

Table 20. Methodologies for navigating trade-offs and making decisions, as adapted for SSbD.

RECOMMENDED ASSESSMENT PRACTICES

Engage stakeholders and document the strategies and tools used to address trade-offs and to assist the decision-making in the SSbD innovation process.

Comparative evaluation matrices. Uses notations such as colouring the results of the assessment for a given endpoint or indicator as Red, Yellow, Green OR +, 0, - or some other ranking scheme.	**Pros:** Useful when the assessor is not making a decision and supports decision-making by other entities. **Cons:** It may be difficult to see a clear preferred alternative if a large number of alternatives were included in the assessment, numerous endpoints/assessment criteria addressed, and if uncertainties and trade-offs abound.
Eliminate the “high” rating: In this strategy, the option is eliminated if it scores “high” on any sensitive aspect (e.g. toxicity endpoint (SSbDH1)).	**Pros:** Any chemical/material with high inherent hazards are not considered a safe alternative. **Cons:** Viable SSbD options might be disregarded**.**
Strict ordering of endpoints: safety and sustainability aspects are strictly ranked such that the highest-ranked governs the overall preference ordering of options.	**Pros:** Useful if specific aspects are of greater concern than others to the decision-maker. **Cons:** This approach requires a strict ordering of the importance of aspects, which may not be supported by all stakeholders.
Equal weighting of endpoints: Each aspect is considered to have equivalent importance, and the trade-off is resolved by assigning a relative weight to the high, medium, and low categories and then adding up the score. The total would indicate the preference ordering of options.	**Pros:** Easily executed. **Cons:** This approach may unnecessarily exclude valuable options and can mask significant weaknesses

Rule-based ranking: Preferences can be ordered by a series of logical statements. The basis for implicit or explicit weighting should be carefully considered before applying a rule-based system to ensure that the organisation's values with respect to the different assessment outcomes are appropriately represented.	**Pros:** An organisation's value system, once codified in the form of these rules, can be consistently applied, which makes the process less prone to an individual's personal judgments or manipulation of the weighting schemes toward otherwise preferred outcomes. **Cons:** Difficult to operationalise if stakeholders cannot weight one aspect over another.
Weighted scoring of aspects: Aspects are given an unequal weight, and the relative score is determined by summing up the weighted scores across the aspects. This approach also requires weighting high, medium, and low the safety and sustainability aspects. This approach will often require the use of analytic decision tools such as multi-criteria decision analysis (MDCA).	**Pros:** Analytic decision tools enable the processing of many endpoints/attributes and varying weights. **Cons:** Requires expertise in the use of analytic decision tools. Use of these tools should be used to support discussion about preferable options, not replace critical and strategic thinking.
Expert–manager judgement: This methodology relies on the application of expert judgement. It replaces the complex scoring or algorithms with a group of experts.	**Pros:** Easily applicable at any stage of innovation, supports the life cycle actors' engagement and collaboration and adds valuable information to the outputs of the assessment. **Cons:** Low level of transparency and variability among experts if not well documented.

Source: OECD, 2021.

13.2. Uncertainty in the SSbD framework

Uncertainty can be considered as a necessary condition of innovation (Jalonen, 2011) whilst innovation as the information-processing activity aims at reducing uncertainty. Therefore, uncertainty considerations should be an integral part of the SSbD implementation and should be considered in the evaluation phase and taken into consideration in the decision making.

How to deal with uncertainty and how to consider it in each of the decision-making steps should be covered to the extent is possible when formulating the decision-making rules.

Sources of uncertainty can be many in the implementation of the SSbD Framework. Uncertainty due to the lack of information about the SSbD system (life cycle) is one of the most important elements together with the uncertainty related to data, sources of data and quality of data for the safety and sustainability assessment. The latter is further described with the safety assessment section (10.3), the environmental sustainability assessment section (11.2), and the socio-economic sustainability assessment section (12.4).

The level of detail of the uncertainty analysis should be coherent with the tiered approach and consistent with the overall scope and purpose of the assessment. With the refinement of the assessment in each iteration new data, information and methods will be incorporated to better characterize uncertainty.

Uncertainty considerations for the assessment should be documented fully and systematically in a transparent manner, including both qualitative and quantitative aspects pertaining to data, methods, scenarios, inputs, models, outputs, sensitivity analysis and interpretation of results.

13.3. Example of a dashboard to visualise SSbD results

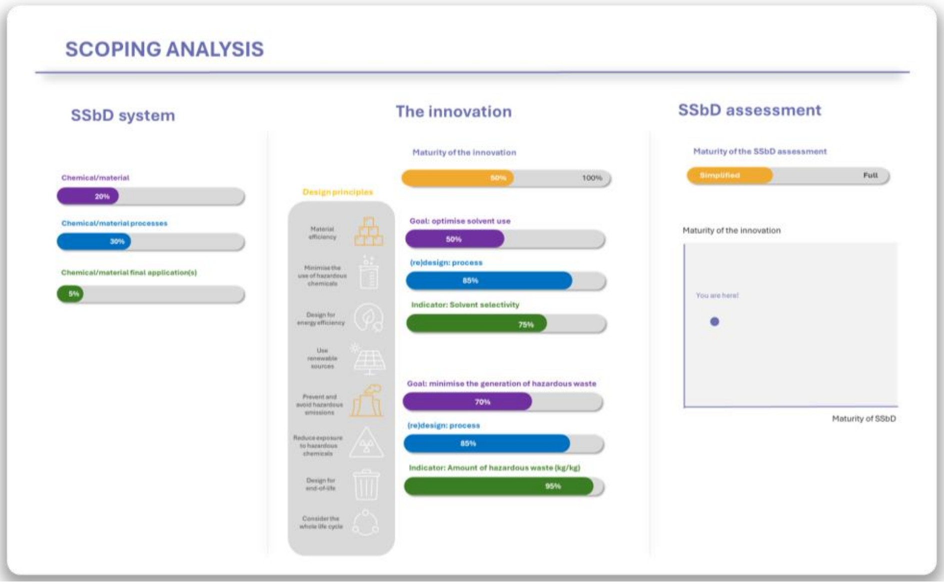
As presented in the previous chapters, the assessment framework of SSbD chemicals/materials entails many aspects that need to be considered individually and then integrated to support decision making when considered appropriate by the SSbD practitioner. To this end, the dashboards below are provided as examples. They show elements and information that should be considered for a comprehensive evaluation of the safety and sustainability aspects and to monitor the innovation process. The dashboards give the practitioner the flexibility to adapt the visualisation of the framework to the maturity of the innovation and allow the inclusion of both qualitative and quantitative outcomes of the assessment (moving from simplified, toward intermediate and full SSbD assessment).

Scoping dashboard. The scoping phase represents the new component introduced in the revised SSbD framework. The dashboard below (Figure 31) provides an example of how the outcomes of the scoping phase can be presented. These elements, which include the definition of the SSbD system, the definition of the innovation (with the example of design principles) and the maturity of the SSbD implementation, will then feed into the subsequent assessment phase. The example of the use of percentages, as shown in the figure, enables practitioners to track the evolution of the innovation (and related completeness of the needed information and data) and also to prepare for a more focused evaluation. This dashboard includes:

- The level of SSbD assessment (simplified, intermediate, full)
- Innovation aspects such as the goal, (re)design and relevant indicators. For illustration the dashboard represents this innovation aspects in the form of (re)design principles
- The maturity of innovation and data quality considerations.

Additional elements of the scoping analysis which are relevant for the assessment could be displayed, for example the sustainability indicators chosen to measure the results of the application of (re)design principles throughout the innovation process.

Figure 31. Example of the dashboard: scoping analysis. The percentage indicates the completeness of data and information needed for the scoping analysis.



Source: Own elaboration

Assessment dashboard. The assessment dashboard offers a comprehensive view of the results from the safety and sustainability assessments. It is designed to be tailored to the maturity level of the innovation – such as TRL (n) - following a tiered approach.

The key elements included in the dashboard are the following:

- Safety assessment (Figure 32): the outcome of the safety assessment is reported for the different elements considered (intrinsic properties, and risk (based on exposure during the manufacturing, processing and use).
- Environmental sustainability assessment (Figure 33): the results are reported for the different elements of the sustainability assessment: the outcome of the LCA is reported for the 16 environmental impact categories
- Socio-economic sustainability assessment (Figure 34): the results are reported for the different impact categories.
- Addressing safe and sustainability from process perspective (Figure 35): to visualize the outcome of the assessment of the indicators for safety and environmental sustainability assessment, focusing on industrial processes/technologies.

The results of the assessments ("Results" in the dashboard images below), can be either qualitative or quantitative. The dashboard helps identifying major hotspots and areas for improvement, while also visualising potential trade-offs within and across the safety and sustainability dimensions. It is accompanied with a traffic light that can be aligned with e.g. a scoring system. This visualisation also allows to identify conflicts between and within the different dimensions of the SSbD, which would not be visible in an aggregated score.

For each of the three dashboards of the evaluation, the following are reported:

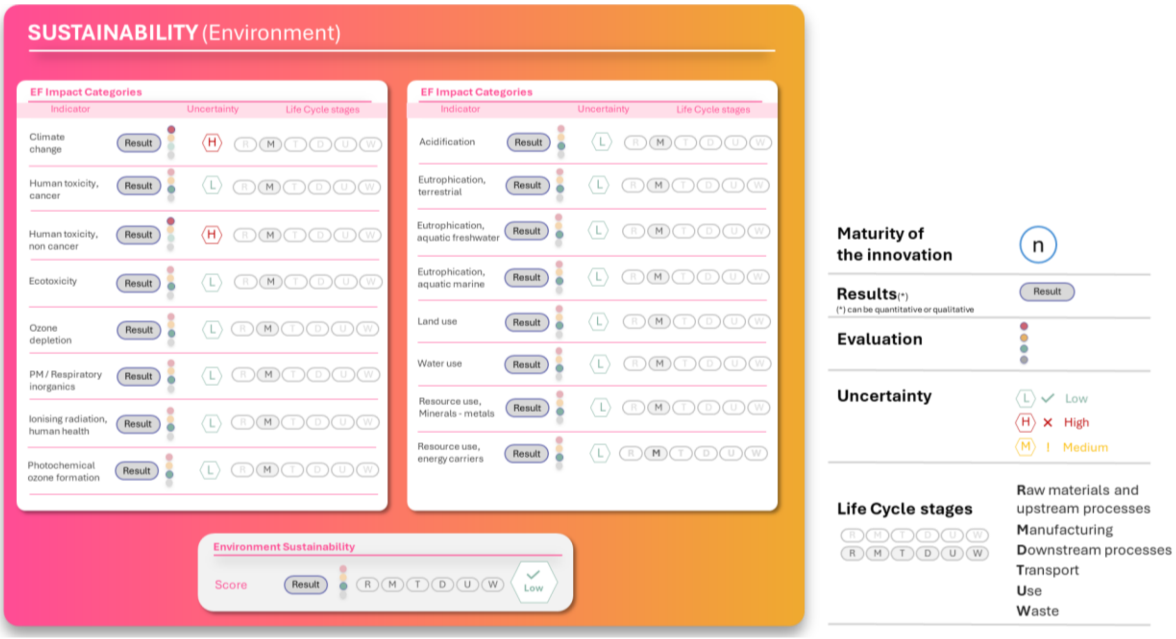
- Level of uncertainty: each result is associated with an uncertainty level that can be assessed through a qualitative or a quantitative approach.
- Life cycle stages: the results of the assessment should include an information related to the life cycle stage considered in the assessment.

The iterative nature of the innovation process, which is reflected in the framework, should allow for progressive integration of elements and increasing completeness.

Figure 32. Example of the dashboard: safety assessment.

Source: Own elaboration

Figure 33. Example of the dashboard: Environmental sustainability assessment.

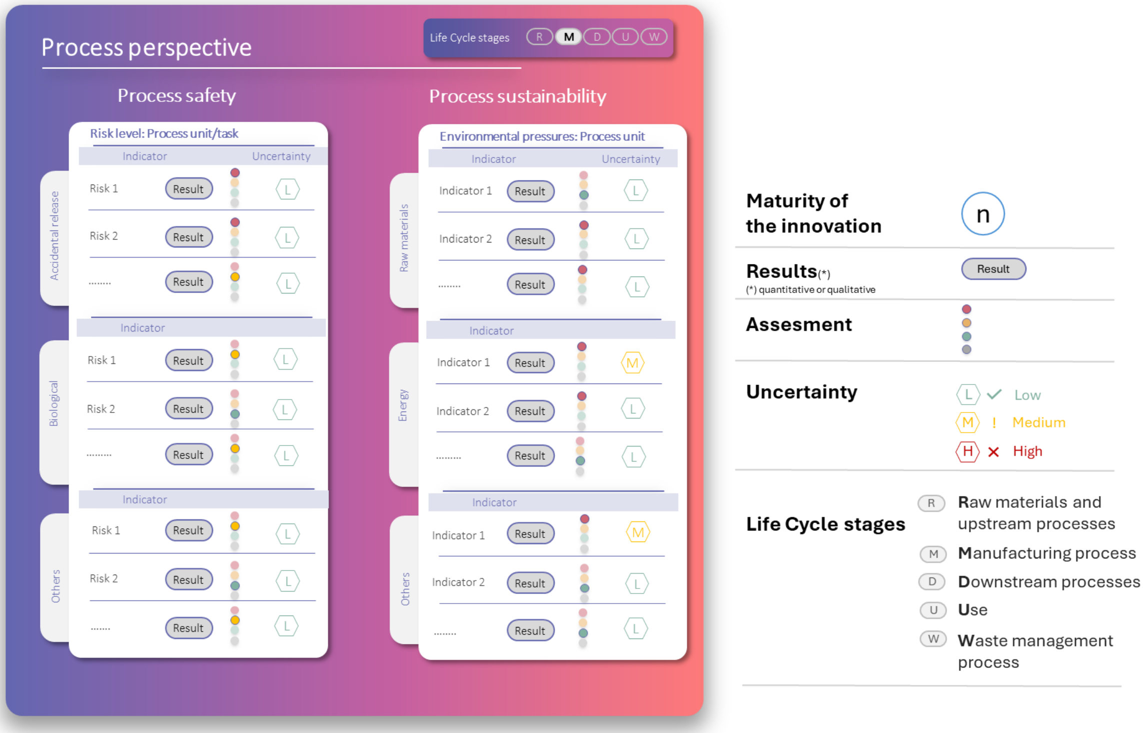


Source: Own elaboration

Figure 34. Example of the dashboard: Socio-economic sustainability assessment.

Source: Own elaboration

Figure 35. Example of the dashboard: Addressing safety and sustainability from the process perspective.



Source: Own elaboration

13.4. Aggregation of results – Multi-Criteria Decision Analysis (MCDA)

The 2022 SSbD framework illustrates options for the aggregation of the SSbD results (Caldeira et al. 2022b).

Aggregation of results from the safety and sustainability assessment may support decision, but in the context of SSbD it is important to note that the use of aggregation methods does not rule out a richer evaluation presenting not only the overall aggregate result, but also the results obtained in other levels of detail. Such information is important to understand the strengths and weaknesses that an aggregate result inevitably might hide and therefore the presentation of the detailed information of the assessment is considered essential, and a key component of the evaluation.

The Box 12 below describes how the MCDA can support decision by aggregating safety and sustainability results, according to the review of Dias et al. (2024) on the use of MCDA to support the evaluation within the SSbD framework.

Box 12. The role of MCDA in supporting SSbD evaluation.

Multi-Criteria Decision Analysis (MCDA) is a well-established field within Operational Research and Decision Theory, aimed at supporting decision-making when multiple, often conflicting, evaluation criteria are involved (e.g. Ishizaka and Nemery, 2013). Its relevance to sustainability assessment has been widely recognized particularly for its ability to combine heterogeneous indicators—ranging from quantitative life cycle impacts to qualitative risk flags—into a coherent, composite understanding of overall performance (e.g. Lindfors, 2021).

Dias et al. (2024) reviewed MCDA applications in the Safe and Sustainable by Design (SSbD) context, highlighting that most existing uses remain comparative, typically evaluating alternatives like fuels or chemical processes. Only a limited number of studies explicitly address both safety and sustainability in relation to chemicals or materials, and many rely on approaches such as weighted averages or Analytic Hierarchy Process (AHP), often without transparent methodological justifications. A major challenge remains the dominance of relative assessments, which contrast with SSbD's need for absolute and standalone evaluations of individual substances.

To overcome this, Dias et al. recommend the adoption of **non-compensatory aggregation methods**, particularly those based on decision rules. These allow the translation of multiple inputs into discrete rating levels without permitting high performance in one area to offset critical weaknesses in another—an essential feature for maintaining safety thresholds and interpretability, especially when qualitative data are involved.

Arias et al. (2024) propose a **composite indicator** to combine safety and sustainability aspects and circularity in emerging technologies, illustrating how MCDA-based approaches can support transparent and structured assessments across diverse dimensions.

It should be remarked that, in the context of the SSbD, the MCDA can also be applied without aggregation, for instance using charts to compare side by side the scores or the ranking of the alternatives compared for multiple indicators[21].

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[21] Other possibilities include outranking, dominance analysis, threshold-based filtering, and partial aggregation, enabling practitioner to explore alternatives, identify non-dominated solutions, and understand value conflicts without collapsing all information into a unique index (Cinelli et al. 2014).

14. Documentation

After each iteration, the SSbD practitioner should document the results of the evaluation, including the scoping exercise, the results of the safety and sustainability assessment as well as the fulfilment of the SSbD framework principles. This is critical to ensure the adherence to the SSbD framework and pivotal to follow the improvements achieved through the innovation process.

The documentation produced could indeed represent a useful repository and summary of the evolution of the innovation process, and be used both for internal (e.g.: between the different functions and hierarchical levels involved in the R&I process) and external communication purposes (e.g.: with the different actors of the life cycle):

- It allows transparency regarding the way the SSbD has been implemented and how its implementation has supported the iterative approach to reduce uncertainties with regard to the level of SSbD “completeness”.
- It ensures traceability of the tiered safety and sustainability assessment, with regards for example to data gaps and identification of hot spots along the innovation process, facilitating the reuse / sharing of the data generated or applied in the assessment.
- It is also an instrument for communication with stakeholders.

The documentation should ideally include:

- A summary stating the important milestones in the innovation, the iterations and conclusion.
- The summary table (Table 21), with the main elements of the scoping analysis, the results of the safety and sustainability assessment.
- The specific tables with the larger description of each of the elements in the summary.
- Table 22 is a checklist of the main scoping analysis elements and options that helps identifying the entry point of the innovation to the SSbD.
- Table 23 is an example of specific tables for stakeholder engagement checklist and recording.

Table 21. Summary table examples with the main elements of the scoping analysis, the results of the safety and sustainability assessment.

	Iteration 1	**Iteration 2**	**…….**	**Last iteration**
Scoping Analysis				
SSbD system	*Process*	*Process and product*		*Chemical, process and product*
Life cycle actors	*Formulator*	*Formulator and user*		*Manufacturer, formulator and user*
Objectives	*Reduce the concentration of the chemical* *Reduce emissions to water and environment in the process*	*Reduce the concentration of the chemical and reduce the exposure in application* *Reduce emissions to water and environment in the life cycle stages* *Energy efficiency*		*Improve the knowledge about the chemical* *Reduce the concentration of the chemical and/or reduce the exposure in application* *Reduce the energy use and emissions to water and environment in the life cycle stages considering EoL.* *Energy efficiency*
(re)design	*Process*	*Process and product*		*Process and product*
Aspects and indicators	*Hazard of components* *Critical water mass (%)* *Biological oxygen demand (g/kg)* *Chemical oxygen demand (g/kg)* *Total organic carbon (g//kg)* *Non-Aqueous Liquid Discharge* (m^3/kg) *Wastewater to treatment* (m^3/kg)	*Mixture classification* *Exposure* *Critical water mass (%)* *Biological oxygen demand (g/kg)* *Chemical oxygen demand (g/kg)* *Total organic carbon (g//kg)* *Non-Aqueous Liquid Discharge* (m^3/kg) *Wastewater to treatment* (m^3/kg) *Energy consumption (kWh/kg or MJ/kg)* *Energy efficiency (%)*		*Risk Characterisation* *Critical water mass (%)* *Biological oxygen demand (g/kg)* *Chemical oxygen demand (g/kg)* *Total organic carbon (g//kg)* *Non-Aqueous Liquid Discharge* (m^3/kg) *Wastewater to treatment* (m^3/kg) *Energy consumption (kWh/kg or MJ/kg)* *Energy efficiency (%)*
Maturity of the innovation	*Low*	*Medium*		*High*
Decision making rules applied	*CLP classification SSbD H2 as minimum requirement for all components* *Energy consumption (kWh/kg or MJ/kg) < X kWh/kg* *Energy efficiency (%)>80%*	*H2 as minimum requirement for the new mixture* *Environmental impact lower than benchmark for climate change and pollution*		*RCR < 1 for the components in the mixture in the process and application* *Environmental impact lower than benchmark for all the impact categories* *Absence of social risk (> medium)*

	Iteration 1	**Iteration 2**	**…….**	**Last iteration**
	Critical water mass (%) *Biological oxygen demand (g/kg)* *Chemical oxygen demand (g/kg)* *Total organic carbon (g//kg)* *Non-Aqueous Liquid Discharge (m^3/kg)* *Wastewater to treatment (m3/kg)* *Exclusion of country-sector combinations with very high social risk*	*Energy consumption (kWh/kg or MJ/kg)* *< X kWh/kg* *Energy efficiency (%)>80%* *Critical water mass (%)* *Biological oxygen demand (g/kg)* *Chemical oxygen demand (g/kg)* *Total organic carbon (g//kg)* *Non-Aqueous Liquid Discharge (m^3/kg)* *Wastewater to treatment (m^3/kg)* *Absence of high social risk in the value chain; minimisation of CRM in the value chain.*		*minimisation of CRM in the value chain* *Selection of option with lowest total costs (incl. Societal costs)*
Results of the safety and sustainability assessment				
Safety assessment	*CLP classification of the ingredients* *Exposure scenarios formulation*	*CLP classification of the mixture* *Exposure scenarios of the application*		*RCR for the specific exposure scenario formulation and product application*
Environmental sustainability assessment	*Identification of the class of performance in relation to the stoichiometry of the reaction, to energy-related aspects (e.g. enthalpy, consumption) and to design principles in comparison with a "proxy" benchmark*	*Identification of the class of performance in relation to the impact results in comparison with a benchmark*		*Identification of the class of improvement in relation to the impact results in comparison with a representative system*
Socio Economic sustainability assessment	*Identification of high-risk country – sectors combination in a simplified value chain and for a subset of social aspects, using secondary data only*	*Identification of high-risk country – sectors combination in a simplified value chain for the full set of social aspects and accounting of CRMs in the value chain.*		*Assessment of social risks and performance, CRM content and total costs of various design options for the full list of socio-economic aspects, using both primary and secondary data*
Summary and conclusion				

NB. The examples reported in the Summary table above are intended to show the type of information that can be included in the documentation, without prejudice the flexibility of the SSbD framework to be used in different scenarios. Source: Own elaboration

Table 22. Example of a scenario building checklist.

Scenario building sheet				Yes/No
SSbD System	Chemical/material	Based on assumptions		
		Based on literature: SDS, databases		
		Based on real data (value chain collaboration)		
	Process	Based on assumption		
		Based on literature: BREF, REACH, e-SDS		
		Based on real data (value chain collaboration)		
	Product	Based on assumption		
		Based on literature: BREF, REACH, e-SDS, sector organisation, use maps, Cons Expo factsheets		
		Based on real data (value chain collaboration)		
Actors in the Life cycle	Actors' involvement	Raw material supplier		
		Chemical manufacturer		
		Formulator		
		Product producer		
		Waste manager		
		Other		
	Degree of involvement	Informative		
		Collaborative		
		Other		
	Type of involvement	NDA		
		Partnership		
		Other		
	Sharing mechanisms	Letter of access		
		Patent license		
		Block chain		
		Other		
	Roles and responsibilities in the SSbD	Safety		
		Sustainability		
		Chemical//material		
		Process(es)		
		Products		
		Other		
Type of innovation	None			
	Incremental			
	Breakthrough			
Objective of the implementation	Safety and sustainability assessment			
	Improvement of	Safety of	Chemical/material	
			Process	
			Product	
		Sustainability of	Chemical/material	
			Process	
			Product	
Type of (re)design considered	None			
	Molecular	Only		
		And process		
		And product		
	Process	Only		
		And product		
	Product	Only		
		And EoL		
Maturity of	Of the (re)design			
	The SSbD implementation			

Source: Own elaboration

Table 23. Stakeholder engagement information and stakeholder information sheet (example).

Stakeholder engagement checklist*	
Purpose	SSbD awareness, collaboration
Mapping	**Stakeholder:** name…. **Type of stakeholder:** worker, supplier, customer…… **Interest:** chemical, process, product, acceptance…. **Influence:** acceptance, Resistance, Neutral **Relevance:** Very High, high, medium, low, very low
Strategy and approach for engagement	How it has been approached • Survey • Meeting • Workshop • Email • Questionnaire
Level of engagement	Informing Consulting Involving Collaboration Partnership
Type of engagement	Mechanism: NDA, Consortia Provide detail on the roles and responsibilities Provide details on the contributions: Scoping, decision rules, alternatives, data, evaluation….
Communication	Frequency Channel Type Of information
Stakeholder information sheet*	
Stakeholder	Name: Type of stakeholder Interest:…. Influence: Relevance:
Purpose of engagement	
Strategy and approach for engagement	
Type of engagement	Mechanism Roles and responsibilities Contributions
Engagement/communication	Frequency Channel Type Of information

*to be completed for each stakeholder involved

Source: Own elaboration

15. Conclusions

This report contains the 2025 revision of the EC-JRC SSbD framework of 2022 (EC, 2022a; Caldeira et al., 2022b), developed in the context of the Chemicals Strategy for Sustainability. This revision is based on: i) the experience gained during the testing period of the SSbD framework (2023 and 2024), ii) the improvement introduced by the methodological guidance and iii) the recognition of innovation as a key enabler of competitiveness and a priority of the European Commission. The revision of the SSbD framework introduces new elements, which aim to facilitate and broaden its application, while keeping the life cycle perspective and the ambition to move towards safe and sustainable by design chemicals and materials.

The scoping analysis contextualises the application of the SSbD framework by defining the system under study and its related (re)design objectives. The outcome of the scoping analysis allows the identification of a scenario that defines the entry point to SSbD and hence helps to tailor the safety and sustainability assessment. The iterative and tiered approach of the SSbD framework is reflected through simplified, intermediate, and full SSbD, accompanied by methodological criteria.

The safety assessment (that merges the previous Steps 1-3) considers the main indicators and criteria applied in Risk Assessment with a broader sense focusing on the possible risks arising with a life cycle perspective. Specifically, a sub-chapter on process-related safety has been added to enhance the comparison among processes, including their different risks and the implications on industrial competitiveness.

The environmental sustainability assessment (previously Step 4) is based on a Life Cycle Assessment methodology and proposes screening assessments when the maturity of the innovation is low. It proposes classes of performances based on a benchmark, i.e. a virtual representative average-impact chemical, to enhance the comparative assessment. A sub-chapter on process-related sustainability has been added to enhance the comparison among processes, including their different environmental impacts and the implications on industrial competitiveness.

The socio-economic sustainability assessment (previously optional Step 5) addresses the social fairness and competitiveness dimensions of the chemical/material supply chain, and includes aspects related to supply chain vulnerabilities and life cycle costs, also linked to risk, governance and financial stability.

The evaluation procedure introduces, as an example, a dashboard where the results of the safety and sustainability assessment and the different aspects are visualised. The visualisation aims to help the practitioner identify possible hotspots and navigate trade-offs along the innovation process.

Furthermore, it is proposed to provide a summary of the results of the application of the SSbD framework within the innovation process via documentation of the application, to ensure transparency in the implementation of the framework and traceability of the results.

List of Abbreviations

AHP	Analytic Hierarchy Process
BPR	Biocidal Products Regulation
BREF	BAT Reference Document
CC	Circular Chemistry
CLP	Classification, Labelling and Packaging
CP	Class of Performance
CRM	Critical Raw Materials
CSRD	Corporate Sustainability Reporting Directive
CSS	Chemicals Strategy for Sustainability
CTUe	Comparative Toxic Unit for ecosystems
CTUh	Comparative Toxic Unit for humans
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EC	European Commission
EF	Environmental Footprint
EIA	Environmental Impact Assessment
eLCC	Environmental Life Cycle Costing
EoL	End of Life
ERC	Environmental Release Category
e-SDS	Extended Safety Data Sheet
ESG	Environmental, Social, Governance
EU	European Union
FD	Framework Directive
GC	Green Chemistry
GE	Green Engineering
GHG	Green House Gas
GR	Golden Rules
GWP	Global Warning Potential
IATAs	Integrated Approaches to Testing and Assessment
IED	Industrial Emission Directive
ILCD	International Reference Life Cycle Data System
ILOSTAT	International Labour Statistics
ISO	International Organization for Standardization
JRC	Joint Research Centre
KOW	Octanol–water partition coefficient
LC50	Lethal Concentration 50%
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCSA	Lyfe Cycle Social Assessment
LCT	Life Cycle Thinking
LD50	Lethal Dose 50%
MCDA	Multi-Criteria Decision Analysis
MCI	Material Circularity Indicator
MEErP	Methodology for Ecodesign of Energy-related Products
MFA	Material Flow Analysis

NAMs	New Approach Methodologies
NMVOC	Non-Methane Volatile Organic Compounds
NOAEC	No Observed Adverse Effect Concentration
NOAEL	No Observed Adverse Effect Level
OECD	Organisation for Economic Co-operation and Development
OEL	Occupational Exposure Limit
OSH	Occupational Safety and Health
PC	Product Category
PEF	Product Environmental Footprint
PM	Particulate Matter
PNEC	Predicted No Effect Concentration
POP	Persistent Organic Pollutant
PROC	Process Conditions
PSILCA	Product Social Impact Life Cycle Assessment
QSAR	Quantitative Structure-Activity Relationship
RCR	Risk Characterisation Ratio
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RMM	Risk Management/Mitigation Measures
RoHS	Restriction of Hazardous Substances
RSA	Reference Scale Approach
SC	Sustainable Chemistry
SDGs	Sustainable Development Goals
SDS	Safety Data Sheet
SEA	Socio-Economic Analysis
SETAC	Society of Environmental Toxicology and Chemistry
SEVESO	Seveso Directive
SHDB	Social Hotspot Database
S-LCA	Social Life Cycle Assessment
S-LCC	Societal Life Cycle Cost
SSbD	Safe and Sustainable by Design
SU	Sector of Use
TF	Technical Function
TP	Transformation Product
TRL	Technology Readiness Level
UNEP	United Nations Environment Programme
UNICEF	United Nations Children's Fund
USDA	United States Department of Agriculture
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable composition, Complex reaction products or Biologicals
VRE	Value-based resource efficiency indicator

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Annexes

Annex 1. List of Definitions and terms used in the SSbD framework

Safety assessment definitions and terms

Advanced material: materials that are designed to have

- new or enhanced properties, and/or
- targeted or enhanced structural features

with the objective to achieve specific or improved functional performance compared to already available materials. This includes both new emerging manufactured materials, and materials that are manufactured from traditional materials. This also includes materials from innovative manufacturing processes that enable the creation of targeted structures from starting materials, such as bottom-up approaches. It is acknowledged that what are currently considered as Advanced Material will change with time.

Article: an object which during production is given a special shape, surface or design which determines its function to a greater degree than does its chemical composition.

DNEL (Derived No-Effect Level): For human health, it represents the level of exposure below which humans are not expected to experience adverse effects.

Downstream user: means any natural or legal person who uses a substance, either on its own or in a mixture, during his industrial or professional activities. A distributor or a consumer is not a downstream user.

Chemical product (or material product): a chemical or material intended for consumers or that is likely -under reasonably foreseeable conditions- to be used by consumers.

Exposure scenario: means the set of conditions, including operational conditions and risk management measures, that describe how the substance is manufactured or used during its life cycle and how controls exposures to humans and the environment are controlled. These exposure scenarios may cover one specific process or use or several processes or uses as appropriate.

Hazard classification: Process in which a given substance or mixture is assigned one of the 28 hazard categories of danger depending on their intrinsic properties in accordance with the criteria specified in CLP. If the substance is not found to be dangerous, according to the said criteria, then it is not classified.

Intermediate: means a substance that is manufactured for and consumed in or used for chemical processing to be transformed into another substance (hereinafter referred to as synthesis).

Intrinsic properties: intrinsic properties of chemicals and materials are characteristics that are inherent to the substance itself, regardless of the amount present. These properties are determined by the chemical composition and structure.

Life cycle of a chemical: encompasses all stages from its creation to its ultimate disposal, including production/manufacturing, storage, transformation, transportation, use, and disposal. The use of chemicals for production is one part of the “use” of a chemical.

Manufacturing: production or extraction of substances in the natural state.

Manufacturer: any natural or legal person manufactures a substance.

Use: any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, production of an article or any other utilisation.

Monomer: means a substance which is capable of forming covalent bonds with a sequence of additional like or unlike molecules under the conditions of the relevant polymer-forming reaction used for the particular process.

PNEC (Predicted No-Effect Concentration): For the environment, it represents the concentration of a substance below which adverse effects on the environment are not expected.

Polymer: means a substance consisting of molecules characterised by the sequence of one or more types of monomer units. Such molecules must be distributed over a range of molecular weights wherein differences in the molecular weight are primarily attributable to differences in the number of monomer units. A polymer comprises the following:

- a simple weight majority of molecules containing at least three monomer units which are covalently bound to at least one other monomer unit or other reactant;
- less than a simple weight majority of molecules of the same molecular weight.

In the context of this definition a 'monomer unit' means the reacted form of a monomer substance in a polymer.

Risk Characterisation Ratio: It's a numerical value that indicates the level of risk associated with a substance's use by comparing the estimated exposure level with a relevant threshold level (DNEL for human health, or PNEC for the environment).

Environmental sustainability assessment definitions and terms

Benchmark: (adjusted definition of the PEF Recommendation) refers to the average environmental performance of the representative chemical.

Chemical grouping level: Groups of chemicals, or groups of chemical production processes that are like each other. For example, a "chemical grouping level" aggregates chemicals according to their chemical structure (e.g. aromatics or alcohols), their chemical process (alkylation, oxidation, etc.).

Class of performance: Starting from the chemical or process grouping levels, and the related benchmark for the representative chemical, the class of performance indicates whether performance is better or worse, for each indicator.

Desired target: a desired value that the innovator aims to achieve, for instance reduction of the resource use by 30% compared to the benchmark, or the status-quo.

Full LCA: it refers to an LCA that follow the recommendation in the PEF.

Functional unit: quantified performance of a chemical/material required to provide a specific function and is the basic requirement for meaningful comparisons in LCA. The functional unit of an LCA can be defined answering to the questions: What is the function/service provided by the chemical/material? To which extent should this function be provided? How long? And how well?

Indicator: an indicator is a pointer or index that indicates something. In LCA analysis it is used to measure the adoption of a specific design principle, or to measure an impact category in LCA. For instance, kgCO2 eq. is an indicator for Climate Change. Another indicator for Climate change may be Global Warning Potential (GWP). Similarly, to measure the level of application of design principles related to circularity, possible indicators that may be utilised are the Value-based resource efficiency indicator (VRE), Material Circularity Indicator (MCI), or the Recycled Content.

Prospective LCA: an LCA methodology suitable to new innovation processes, which estimate the associated environmental impacts before the new / redesigned chemical or material is placed on the market, i.e., referring to ex-ante evaluations.

Reference flow: the amount of a chemical/product that is needed to fulfil the functional unit.

Reference: a standard value against which any comparison may be made. In the context of the SSbD, the reference can be either a benchmark, a target, or the status quo of the specific innovation.

Representative system: SSbD system – that may be virtual or real – used for the comparative assessment as the initial starting point of the innovation, representing the current situation to be improved upon. The information of the representative system comes from either literature or engagement with the actors of the life cycle.

Simplified LCA: it is the full LCA with several assumptions and simplifications because some aspects are unknown.

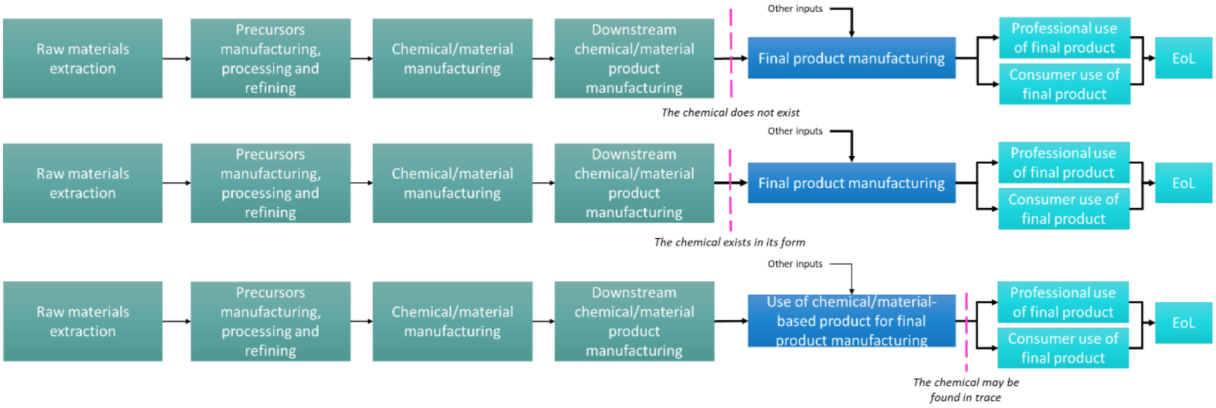
Intermediate LCA: it comprises the iterative modelling of the LCA that goes from a simplified LCA to a more complete assessment but lacking the full detail of a PEF-compliant LCA or equivalent.

Tiered LCA: this is the overall approach applicable in the context of the SSbD framework, so called because it comprises the progressively more developed LCA tiers of: a simplified LCA, an intermediate LCA and finally a full LCA.

Use phase: The use phase of the life cycle of a chemical/material is shown in Figure 36. Based on its function and its final forms, the downstream final product manufacturing and the use phase can be different. The figure comes from various sources such as REACH and PEF. According to REACH, end uses of a substance are: use at industrial sites, widespread use by professional workers, and consumer use (ref. R12). According to PEF, the use phase (of a product) is usually referred to as being the widespread use by professional workers, or consumer use. However, PEF studies have been usually performed for products which do not require downstream manufacturing/production processes. Note that chemicals and materials, once produced, may be used at an industrial site for further manufacturing processes, leading to the final product. For the purposes of REACH, “use” means any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, production of an article or any other utilisation.

“Use” at industrial sites includes: (1) chemical reaction, hence (if it is fully used up during the chemical reaction) it will not exist anymore; (2) encapsulation in a product; (3) use of the chemical as an ancillary input for other processes, and hence it may be found in the emission flows (water, air or waste). In LCAs of chemicals, the use phase should be consistent with the general definition of “use phase” of an LCA for products, to guarantee a fair comparison. Hence, here, the “use phase” includes widespread use by professional workers as well as consumer use. An additional life cycle stage for LCA of chemicals is needed to describe uses at industrial sites, which may be referred to as the “downstream manufacturing phase” (i.e. formulation).

Figure 36. Life cycle option of a chemical/material according to its downstream processes, i.e. final product manufacturing and use phases.



Source: Own elaboration

Social and economic sustainability related definitions and terms

Critical Raw Materials (CRMs): raw materials of high importance to the economy for the EU that are associated with high risk of supply disruption**.**

Due diligence: the process through which organisations identify, consider, and address the potential environmental and social impacts related to their activities and the ones of their business relationships, as an integral part of their decision-making and risk management system.

Externality: consequence of an activity that affects interested parties other than the organisation undertaking the activity, for which the organisation is neither compensated nor penalised through markets or regulatory mechanisms. If a policy is already in place that will cause for example a release to be priced in the near future (e.g. a CO_2 tax) then this can be referred to as “soon-to-be-internalised externality” (see also eLCC). Note that for the latter case internalisation might not be complete.

Life Cycle Costing (LCC): as the economic pillar of Lyfe Cycle Social Assessment (LCSA), is a methodology for calculating the costs (and, if extended, also benefits) over the life cycle of a product directly borne by one or more actors involved (supplier, producer, user/consumer, end-of-life actor). When applied at product level, LCC generally aims to estimate costs associated with the production, commercialisation, use, and end-of-life, i.e. by default extending beyond the producing firm’s own boundaries.

Primary data: information about a unit process or an activity obtained from a direct measurement, or a calculation based on direct measurements at its original source. In Social LCA, primary data corresponds to company or site-specific information which describes the behaviour of the organisation(s) that can be measured only referring to specific and real situation.

Reference Scale Approach (RSA): in the social impact assessment phase, the RSA assesses social performances and risks based on pre-defined, specific reference points of expected activity. The approach does not establish a direct link between the activity and long-term impacts but rather estimates the likely magnitude and significance of potential impacts in the assessed product system.

Reference scale: Reference scales are ordinal scales, quantitative (i.e. from 1 to 5) or qualitative (i.e. from very low to very high), which set known intervals and thresholds, corresponding to levels of risk/performance.

Secondary data: information obtained from sources other than primary data (databases, literature, etc.). In Social LCA secondary data consist of statistics and database information that describe the likelihood that a certain social topic might be relevant, and are used for assessing the social risks, especially in the background processes. Consequently, social risks can be measured according to more general information and statistics which are generally available at country, regional or sector level.

Social hotspot: processes, activities or geographical locations along the product's life cycle where a social issue (as positive or negative performance) and/or social risk is likely to occur.

Social Life Cycle Assessment (S-LCA): A social and socio-economic Life Cycle Assessment (S-LCA) is a social impact (actual and potential impacts) assessment technique that aims to assess the social and socio-economic aspects of products and their positive and negative impacts along their life cycle encompassing extraction and processing of raw materials, manufacturing, distribution, use, re-use, maintenance, recycling, and final disposal.

Social performances refer to the principles, practices, and outcomes of organisations' relationships with people, organisations, institutions, communities, and societies in terms of the deliberate actions of businesses toward these stakeholders as well as the unintended externalities of business activity measured against a known standard.

Social impacts: Social impacts are consequences of positive or negative pressures on social endpoints of area of protection (i.e. well-being of stakeholders).

Social risk is a measure of the likelihood of negative effects only (damage, injury, loss) that may be avoided through preventive actions.

Social sustainability: identifying and managing impacts, both positive and negative, on people (stakeholders).

Societal costs: total costs to society of an economic activity, encompassing both private costs (directly incurred by producers and consumers) and external costs (those imposed on third parties not directly involved in the activity). In the SSbD context, societal costs are calculated through monetisation of LCA impact results.

Stakeholder: person or organisation that can affect, be affected by, or perceive itself to be affected by a decision or activity).

Annex 2. Examples of the scoping analysis

Table 24. Example of the definition of the system(s) under study.

Chemical/material	Chemical A	Material A
Existing / New	Existing	New
Used by	Downstream manufacturers	Downstream manufacturers
Final form	Encapsulated or transformed (depends on the downstream use)	Unknown
Function	plasticiser	insulation
Known application(s)	Several, such as packaging, etc.	Several but not defined
Selected application	Not defined yet	Not defined
Processes involved in the manufacturing		
Information on precursors (name, origin, etc.)	Fossil based	Precursors decided but not the origin because at lab scale
Information on downstream customers		Unknown
Safety issues	None	Unknown
Environmental issues	Generation of by-products	Unknown
Circularity information	Unknown – to be investigate	Unknown
Availability of data for the assessment	Data from our responsibility + partial data from the other actors of the value chain + the remaining data gap from db+literature review	No data -> main sources of data are databases, literature review + experiments

Source: Own elaboration

Table 25. Example of the description of the innovation.

Chemical	Chemical A	Material A
Type of (re)design	Process	Molecular
Maturity of innovation	TRL 9 (high)	Stage-gate 2 (low)
Number of alternatives	3	20
Goal of the innovation	Find an alternative process to improve the environmental issues identified by using biobased precursors	Introduce a new chemical with a new function
Key indicators/aspects for the SSbD assessment	Reduction of the by-products generation	Not defined, overall SSbD assessment to evaluate the new material
Selected SSbD principles and related indicators	SSbD7, SSbD8	All SSbD principles
Target values for the indicators	Recycled content from 0% to 30%	No target
Reference for the evaluation	Target for the indicators with a target, the rest the status-quo	Benchmark of the chemical in the market
Availability of data for the assessment	Data from our responsibility + partial data from the other actors of the value chain + the remaining data gap from db+literature review	No data -> main sources of data are databases, literature review + experiments

Source: Own elaboration

Annex 3. Design principles and examples of indicators

The SSBD can start with the application of design principles towards safer and more sustainable solutions. The literature provides a number of these principles, such as, for example, GC: Green Chemistry Principle (Anastas and Warner, 1998), GE: Green Engineering Principles (Anastas and Warner,2003), SC: Sustainability Chemistry Criteria (UBA, 2009), GR: UBA Golden Rule (UBA, 2016), CC: Circularity Chemistry Principles (Keijer et al. 2019). The list below provides an overview of the design principles which are often applied to steer innovation, and possible indicators to assess them.

Table 26. List of SSbD design principles and associated definition, and examples of actions and indicators that can be used in the design phase.

SSbD principle (based on)	Definition	Examples of Actions	Examples of indicators related to the SSbD principle
SSbD1 Material efficiency (GC2, CC2, GC8, GC9, GC5, CC5, GC1, SC2)	Pursuing the incorporation of all the chemicals/materials used in a process into the final product or full recovery inside the process, thereby reducing the use of raw materials and the generation of waste	- Maximise yield during reaction to reduce chemical/material consumption - Improve recovery of unreacted chemicals/materials - Optimise solvent for purpose (amount, typology and recovery rate) - Select materials and processes that minimise the generation of waste - Minimise the number of chemicals used in the production process - Minimize waste generation - Identify occurrence of use of Critical Raw Material[22], towards minimizing or substituting them	- Net mass of materials consumed (kg per kg of product) - Reaction Yield - Atom Economy - Material Intensity index - Reaction efficiency (i.e. E-factor (%)) - Purity of recovered solvent (%) - Solvent selectivity [-] - Yield of extraction (%) - Water consumption (m^3/kg) - Recycling efficiency/recovery rate (%) - Total amount of waste (kg/kg) - Amount of waste to landfill (kg/kg) - Critical Raw Material presence (yes/no)
SSbD2 Minimise the use of hazardous chemicals/materials (GC3, SC1, GR1, GC4, GE1, GR3, GC5)	Preserve functionality of products while reducing or avoiding use of hazardous chemicals/materials where possible	- Reduce and/or eliminate hazardous chemicals/materials in manufacturing processes - Verify possibility of using hazardous chemicals/materials in closed loops when they cannot be reduced or eliminated - Eliminate hazardous chemical/materials in final products	- Biodegradability of manufactured chemical/material - Classification of raw chemicals/materials as SVHC (yes/no)

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[22] https://ec.europa.eu/growth/sectors/raw-materials/areas-specific-interest/critical-raw-materials_en

SSbD principle (based on)	**Definition**	**Examples of Actions**	**Examples of indicators related to the SSbD principle**
SSbD3 Design for energy efficiency (GC6, CC4, GE4, GE5, CC8, GE8, GE10, GE3, GR7, GC8, GC9, CC10)	Minimise the overall energy used to produce a chemical/material in the manufacturing process and/or along the supply chain	Select and / or develop (production) processes considering: - Alternative and lower energy intensive production/separation techniques - Optimize energy efficiency of solvent recovery - Maximise energy re-use (e.g. heat networks integration and cogeneration) - Fewer production steps (e.g. applying lean thinking) - Use of catalysts, including enzymes - Reduce inefficiencies and exploit available residual energy in the process or select lower temperature reaction pathways	- Boiling temperature (°C) - Heat of vaporisation (MJ/kg) - Energy consumption (kWh/kg or MJ/kg) - Energy efficiency (%) - Solvent selectivity [-] - Yield of extraction (%)
SSbD4 Use renewable sources (GC7, CC3, GE12, SC2)	Target resource conservation, either via resource closed loops or using renewable material / secondary material and energy sources	Verify the possibility of selecting feedstocks that: - are renewables or secondary materials - do not create land competition and / or processes that: - use energy resources which are renewable and with low carbon emissions	- Renewable or fossil feedstock? (yes/no) - Recycled content (%) - Share of Renewable Energy (%)
SSbD5 Prevent and avoid hazardous emissions (GE11, GC11, CC6, SC2)	Apply technologies to minimise and/or to avoid emission of hazardous pollutants into the environment	Select materials and / or processes that: - minimise the generation of hazardous waste - minimise generation of emissions (e.g. Volatile Organic Compounds, acidifying and eutrophying pollutants, heavy metals etc.)	- Critical air mass (%) - Critical water mass (%) - Biological oxygen demand (g/kg) - Chemical oxygen demand (g/kg) - Total organic carbon (g//kg) - Non-Aqueous Liquid Discharge (m^3/kg) - Wastewater to treatment (m^3/kg) - Amount of hazardous waste (kg/kg)
SSbD6 Reduce exposure to hazardous substances (GC12, GR4, SC1)	Reduce or eliminate exposure to chemical/material hazards from processes as much as possible. Chemicals/materials which require a high degree of risk management should be avoided where possible and the best technology should be used to avoid exposure along all the life cycle stages	- Eliminate or minimise risk through reduction of the use of hazardous substances - Analyse and avoid as much as possible the use of substances identified as SVHC - Consider sector-specific regulations - Reduction and/or elimination of hazardous substances in manufacturing processes	- Biodegradability of manufactured chemical/material (yes/no) - Classification of raw chemicals/materials as SVHC (yes/no)
SSbD7 Design for end-of-life (GC10, CC1, CC7, GE11, CC9, GE9, GE6, GE7)	Design chemicals/materials in a way that, once they have fulfilled their function, they break down into products that do not pose any risk to the environment/humans.	- Avoid using chemical/materials that hamper the recycling processes at end-of-life - Select processes (and material) that minimise the generation of waste. - Select materials that are (where appropriate):	- Recyclability rate (%) - Durability (years) - Disassembly/reparability design (yes/no) - Collection rate (%) - Sorting rate (%) - Time for disassembly (%) - Reusability rate (%)

SSbD principle (based on)	**Definition**	**Examples of Actions**	**Examples of indicators related to the SSbD principle**
	Design for preventing the hindrance of reuse, waste collection, sorting and recycling/upcycling. Design to promote circularity	- more durable (extended life and less maintenance) - easy to separate and sort - valuable after their use (commercial after life) - truly biodegradable for uses which unavoidably lead to dispersion into the environment or wastewater	
SSbD8 Consider the whole life cycle (GE6, GR2, SC3, GR6, GR8)	Apply the other design principles thinking through the entire life cycle, from supply chain of raw materials to the end-of-life in the final product	Consider for example: - Using reusable packaging for the chemical/material under assessment and for chemicals/materials in its supply chain - Consider the most likely use of chemical/material and if there is the possibility to recycle it -. Energy-efficient logistics (i.e. reduction of transported quantities, change in mean of transport) - Reducing transport distances in the supply chain	- Recyclable? (yes/no) - Disassembly/reparability design (yes/no) - Durability (years) - Value-based resource efficiency indicator (VRE) - Material Circularity Indicator (MCI) - Biodegradability of manufactured chemical/material (yes/no)
SSbD9 Ensure responsible sourcing and minimise social risks	Avoid that procurement practices are linked with severe human rights and labour rights abuses, as well as other unethical practices.	Perform a suppliers' assessment based on social performance and risk. Include ESG performance as a criterion for suppliers' selection Scrutinise suppliers operating in conflict-affected and high-risk areas Monitor suppliers' compliance with labour and human rights standards. Map the supply chain to identify and address high-risk regions and supplier	- Share of materials sourced from certified responsible schemes (e.g. Initiative for Responsible Mining Assurance (IRMA); Conflict Free Smelter Programme (CFSP); Fairmined) - Share of suppliers located in high-risk countries for labour/human rights - Share of suppliers with third-party sustainability certifications

Source: adapted from Caldeira et al., 2022b

SSbD7: Design for End-of-Life. Indicators to assess circularity

In the SSbD framework (Caldeira et al., 2022b) the collection, sorting and reuse and preparing for reuse are not supported by corresponding example indicators specifically for the SSbD7 Design for end-of-life. This apparent lack of some example indicators could be attributed to the interlinkage between design principles, as in the case of the SSbD1 Material efficiency, that could be assessed with the indicators Recycling efficiency/recovery rate (%).

The proposed list of indicators is not meant to be exhaustive nor representative for specific cases (e.g. the indicator Purity of recovered solvent (%) could be considered more appropriate quantitative indicator for the step "Reuse and preparation for reuse"), instead the list of indicators aims to guide the assessment of the SSbD7 in a more structured manner based on a stepwise approach.

Table 27. Example indicators for the SSbD7 Design for the end-of-life.

End-of-life step	Type of indicator	Indicat	Definition	Assessment method	New/already present
Collection	Qualitative	Yes/No	Is the chemical/material under assessment possibly collected considering it in the final product?	Check literature e.g. material flow analysis (MFA) reports and Eurostat database[23]	New
Collection	Mass based	Collection rate (%)	Expected percentage of recovered material/chemical from the sorting of a chemical/material at the end-of-life of the product.	Estimated using data from literature and other relevant sources. Consider using data geographically consistent with the market of the assessed chemical/material.	New
Sorting	Qualitative	Yes/No	Is the chemical/material under assessment possibly sorted considering it in the final product?	Check literature e.g. material flow analysis (MFA) reports and Eurostat database	New
Sorting	Mass based	Sorting rate (%)	Expected percentage of recovered material/chemical from the sorting of a chemical/material at the end-of-life of the product.	Estimated using data from literature and other relevant sources. Consider using data geographically consistent with the market of the assessed chemical/material.	New
Disassembly	Qualitative	Yes/No	Consider if the chemical/material, in its final application, is reparable or easily disassembled from the rest of the product for substitution (e.g. a polymer component that can be glued if broken or substituted with a new one without replacing the whole product).	[-]	Already present
Disassembly	Time based	Time for disassembly (hr)	Time needed to recover the chemical/material from the product in dismantling operations	Estimated using data from literature and other relevant sources. Consider using data geographically consistent with the market of the assessed chemical/material.	New
Reuse and preparation for reuse	Qualitative	Yes/No	Is the chemical/material under assessment possibly used again without requiring any reprocessing or treatment[24] considering it in the final product?	Check literature e.g. material flow analysis (MFA) reports	New
Reuse and preparation for reuse	Mass based	Reusability rate (%)	Expected percentage of recovered chemical/material that can be used again without requiring any reprocessing or treatment	Estimated using data from literature and other relevant sources. Consider using data geographically consistent with the market of the assessed chemical/material.	New

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[23] https://ec.europa.eu/eurostat/data/database

[24] Definition adapted from “reusability” as in Bachmann, T.M., Hackenhaar, I.C., Horn, R., Charter, M. Gehring, F., Graf, R., Huysveld, S., Alvarenga, R.A.F. (2021). Orienting Project D1. 4 Critical evaluation of material criticality and product-related circularity approaches. https://orienting.eu/wp-content/uploads/2022/01/D1.4_Criticality_circularity_Final-1.pdf (accessed 09.05.22)

End-of-life step	Type of indicator	Indicator	Definition	Assessment method	New/already present
Recycling	Qualitative	Yes/No	Is the chemical/material under assessment recyclable considering it in the final product?	Check e.g. the product or chemical's physicochemical properties and the last type of use of the product/chemical.	Already present
Recycling	Mass based	Recyclability rate (%)	Expected percentage of recovered material/chemical from the recycling of a chemical/material at the end-of-life.	Estimated using data from literature and other relevant sources. Consider using data geographically consistent with the market of the assessed chemical/material.	New for SSbD 7 (previously mentioned for SSbD 1)

Source: Own elaboration

Annex 4. European Regulatory Frameworks linked with chemical safety

Table 28. Examples of European Union legislation established to assess Chemical safety, Workplace safety, Environmental Safety, Process safety and Product safety.

	Acronym	Legislation	Purpose	Area of application
Chemicals	CLP	Regulation (EC) 1272/2008	Harmonisation of criteria for classification, labelling, and packaging of chemicals and mixtures.	Applies to manufacturers, importers, downstream users and distributors of substances and mixtures.
	REACH	Regulation (EC) 1907/2006	Ensures a high level of human and environmental protection from chemical risks; promotes alternative test methods.	Covers all chemical substances; applies to manufacturers, importers, and downstream users.
	POP	Regulation (EU) 2019/1021	Controls and eliminates the use of persistent organic pollutants.	Applies to production, use, and disposal of POPs.
Processes	Water FD	Directive (EC) 2000/60	Establishes the EU framework for water protection and sustainable use.	Applies to all inland surface waters, transitional waters, coastal waters, and groundwater.
	Waste FD	Directive (EC) 2008/98	Sets the legal framework for waste management in the EU.	Applies to prevention, reuse, recycling, and disposal of waste.
	AIR	Directive (EC) 2008/50	Defines and establishes objectives for ambient air quality to protect human health and the environment.	Covers ambient air quality and cleaner air policies.
	SEVESO	Directive (EU) 2012/18	Prevention of major accidents involving dangerous substances and limiting their consequences.	Applies to sites where dangerous substances are present in significant quantities.
	IED	Directive (EU) 2024/1785	Minimisation of pollution from various industrial sources.	Applies to large industrial installations.
	OSH	Directives (EC) 98/24, 2004/37, 2000/54	Ensuring worker safety and health protection, especially from chemical agents at work (98/24/EC), and specifically carcinogens or mutagens (2004/37/EC), and biological agents (2000/54/EC)	Applies to all workplaces within the EU.
	EIA	Directive (EU) 2014/52	Assessment of the effects of certain public and private projects on the environment	Applies to certain industrial sectors and plants in the EU.
Products	GPSD	Directive (EC) 2001/95	Ensuring that only safe consumer products are placed on the market.	Applies to all consumer products not covered by sector-specific legislation.
	TSD	Directive (EC) 2009/48	Ensuring safety of toys for children under normal or reasonably foreseeable conditions of use.	Applies to all toys marketed in the EU.
	FCMR	Regulation (EC) 1935/2004	Ensuring that materials in contact with food do not release harmful substances.	Covers all materials and articles intended to come into contact with food.
	MDR	Regulation (EU) 2017/745	Ensuring the safety and performance of medical devices.	Applies to medical devices and their accessories placed on the EU market.

Acronym	Legislation	Purpose	Area of application
CPR	Regulation (EC) 1223/2009	Ensuring the safety of cosmetic products and free movement within the EU market.	Applies to all cosmetic products placed on the EU market.
BPR	Regulation (EU) 528/2012	Ensuring that biocidal products are safe to use, and protecting humans, animals, and the environment.	Applies to the placing on the market and use of biocidal products.
PPPR	Regulation (EC) 1107/2009	Ensuring that plant protection products are safe to use.	Covers placing on the market and use of pesticides.
VMPR	Regulation (EU) 2019/6	Ensuring the availability, safety, and efficacy of veterinary medicines.	Applies to the manufacture, authorisation, and marketing of veterinary medicinal products.
MPHD	Directive (EC) 2001/83	Ensuring the safety, efficacy, and quality of medicinal products for human use.	Applies to all medicinal products for human use in the EU.
RoHS	Directive (EU) 2011/65	Restricting the use of hazardous substances in electrical and electronic equipment.	Applies to manufacturers and importers of EEE.
BATT	Directive (EC) 2006/66	Regulating the collection, recycling, and disposal of batteries and accumulators.	Applies to all types of batteries and accumulators.
EoLV	Directive (EC) 2000/53	Reducing the environmental impact of end-of-life vehicles.	Covers collection, treatment, and recycling of vehicles.

Source: Own elaboration

Annex 5. Description of the Environmental Footprint 3.1 Impact Categories

Climate change

This indicator refers to the increase in the average global temperatures as result of greenhouse gas (GHG) emissions. The greatest contributor is generally the combustion of fossil fuels such as coal, oil, and natural gas. The global warming potential of all GHG emissions is measured in kilogram of carbon dioxide equivalent (kg CO_2 eq), namely all GHG are compared to the amount of the global warming potential of 1 kg of CO_2.

Ozone depletion

The stratospheric ozone (O_3) layer protects us from hazardous ultraviolet radiation (UV-B). Its depletion increases skin cancer cases in humans and damage to plants. The potential impacts of all relevant substances for ozone depletion are converted to their equivalent of kilograms of trichlorofluoromethane (also called Freon-11 and R-11), hence the unit of measurement is in kilogram of CFC-11 equivalent (kg CFC-11 eq).

Human toxicity, cancer effects

This indicator refers to potential impacts, via the environment, on human health caused by absorbing substances from the air, water and soil. Direct effects of products on human health are currently not measured. The unit of measurement is Comparative Toxic Unit for humans (CTUh). This is based on a model called USEtox.

Human toxicity, non-cancer effects

This indicator refers to potential impacts, via the environment, on human health caused by absorbing substances from the air, water, and soil. Direct effects of products on human health are currently not measured. The unit of measurement is Comparative Toxic Unit for humans (CTUh). This is based on a USEtox model.

Particulate matter

This indicator measures the adverse impacts on human health caused by emissions of Particulate Matter (PM) and its precursors (e.g. NOx, SO2). Usually, the smaller the particles, the more dangerous they are, as they can go deeper into the lungs. The potential impact of is measured as the change in mortality due to PM emissions, expressed as disease incidence per kg of $PM_{2.5}$ emitted.

Ionising radiation

The exposure to ionising radiation (radioactivity) can have impacts on human health. The Environmental Footprint only considers emissions under normal operating conditions (no accidents in nuclear plants are considered). The potential impact on human health of different ionising radiations is converted to the equivalent of kilobequerels of Uranium 235 (kg ^{235}U eq).

Photochemical ozone formation

Ozone (O_3) on the ground (in the troposphere) is harmful: it attacks organic compounds in animals and plants, it increases the frequency of respiratory problems when photochemical smog (“summer smog”) is present in cities. The potential impact of substances contributing to photochemical ozone formation is converted into the equivalent of kilograms of Non-Methane Volatile Organic Compounds (e.g. alcohols, aromatics, etc.; kg NMVOC eq).

Acidification

Acidification has contributed to a decline of coniferous forests and an increase in fish mortality. Acidification can be caused by emissions to the air and deposition of emissions in water and soil. The most significant sources are combustion processes in electricity, heat production, and transport. The more sulphur the fuels contain the greater their contribution to acidification. The potential impact of substances contributing to acidification is converted to the equivalent of moles of hydron (general name for a cationic form of atomic hydrogen, mol H^+ eq).

Eutrophication, terrestrial

Eutrophication arises when substances containing nitrogen (N) or phosphorus (P) are released to ecosystems. These nutrients cause a growth of algae or specific plants and thus limit growth in the original ecosystem. The potential impact of substances contributing to terrestrial eutrophication is converted to the equivalent of moles of nitrogen (mol N eq).

Eutrophication, freshwater

Eutrophication impacts ecosystems due to substances containing nitrogen (N) or phosphorus (P), which promotes growth of algae or specific plants. If algae grow too rapidly, it can leave water without enough oxygen for fish to survive. Nitrogen emissions into the aquatic environment are caused by fertilisers used in agriculture, but also by combustion processes whereas phosphorus emissions are due to sewage treatment plants for urban and industrial effluents and leaching from agricultural land. The potential impact of substances contributing to freshwater eutrophication is converted to the equivalent of kilograms of phosphorus (kg P eq).

Eutrophication, marine

Eutrophication in ecosystems happens when substances containing nitrogen (N) or phosphorus (P) are released to the ecosystem. As a rule, the availability of one of these nutrients will be a limiting factor for growth in the ecosystem, and if this nutrient is added, the growth of algae or specific plants will increase. For the marine environment this will be mainly due to an increase of nitrogen (N). Nitrogen emissions are caused largely by the agricultural use of fertilisers, but also by combustion processes. The potential impact of substances contributing to marine eutrophication is converted to the equivalent of kilograms of nitrogen (kg N eq).

Ecotoxicity, freshwater

This indicator refers to potential toxic impacts on an ecosystem, which may damage individual species as well as the functioning of the ecosystem. Some substances tend to accumulate in living organisms. The unit of measurement is Comparative Toxic Unit for ecosystems (CTUe). This is based on USEtox model.

Land use

Use and transformation of land for agriculture, roads, housing, mining or other purposes. The impacts can vary and include loss of species, of the organic matter content of soil, or loss of the soil itself (erosion). This is a composite indicator measuring impacts on four soil properties (biotic production, erosion resistance, groundwater regeneration and mechanical filtration), expressed in points (Pts)

Water use

The abstraction of water from lakes, rivers or groundwater can contribute to the ‘depletion’ of available water. The impact category considers the availability or scarcity of water in the regions where the activity takes place, if this information is known. The potential impact is expressed in cubic metres (m3) of water use related to the local scarcity of water.

Resource use, fossils

The earth contains a finite amount of non-renewable resources, such as fossil fuels like coal, oil and gas. The basic idea behind this impact category is that extracting resources today will force future generations to extract less or different resources. For example, the depletion of fossil fuels may lead to the non-availability of fossil fuels for future generations. The amount of materials contributing to resource use, fossils, are converted into MJ.

Resource use, minerals and metals

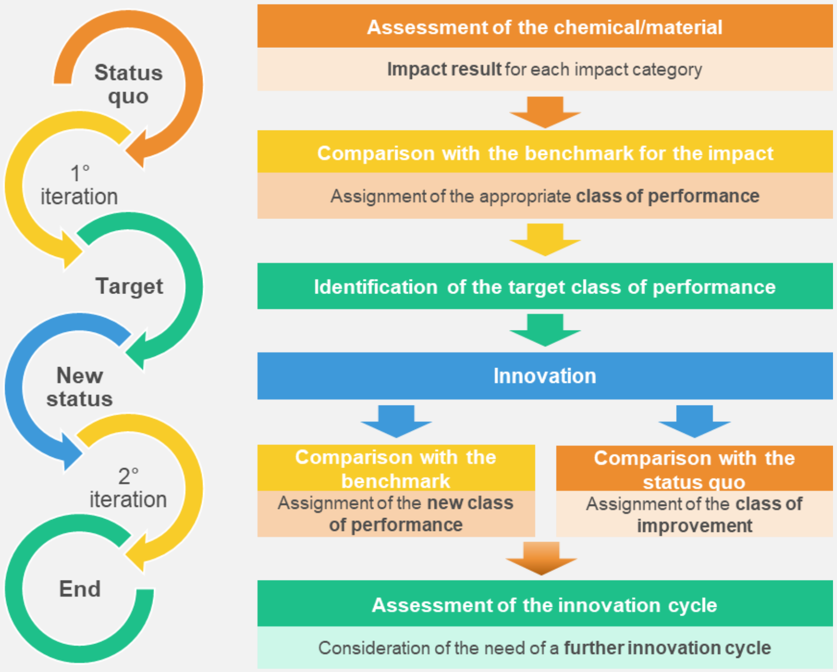
This impact category has the same underlying basic idea as the impact category resource use, fossils (namely, extracting a high concentration of resources today will force future generations to extract lower concentration or lower value resources). The amount of materials contributing to resource depletion are converted into equivalents of kilograms of antimony (kg Sb eq).

Annex 6. Example of evaluation with references for medium/high TRL

The **benchmark**, representative of the overall state of the art, aims at providing more robust basis for the evaluation of the chemical/material under assessment; therefore, it is recommended to perform the comparison against the benchmark, when possible (see Box 13 for an example of application of references in the context of the evaluation).

Box 13. Example of evaluation with references for medium/high TRL.

The image below shows an example of how the references can be used **throughout the innovation for medium/high TRL.** Rationales for the sequence of steps are provided hereafter. In the example, the impact results (status quo) of the chemical/material under assessment are calculated and compared first with the benchmark for the impact, to identify the appropriate class of performance (1° iteration of the evaluation). The comparison with the **benchmark** defined ensures an objective assessment of the chemical/material under assessment in relation to the state of the art, from which then it is possible to identify the aimed **target (i.e. a certain class of performance).** After the innovation process, the new status achieved is proposed to be compared with the benchmark in a 2° iteration, which allows to identify any advancements towards the target. If the outcome of the comparison shows that no advancements are reached (i.e. there is no change in the assignment of the class of performance), this result does not necessarily imply that an improvement did not occur. Therefore, the comparison with the status quo to identify the class of improvement could complement in parallel the first comparison. The outcomes of the comparisons in the 2° iteration are subsequently jointly assessed towards the need of a further innovation cycle.



Source: Own elaboration

Annex 7. Further aspects on data quality

When analysing the data used it is essential to ensure high-quality data in evaluating the sustainability of chemicals, materials, and products under the SSbD framework. For example, in LCA and Environmental Footprint, **data quality** issues are a concern. Data quality aspects are mentioned in the ISO 14040:2006 and ISO 14044:2006 standards, but only qualitatively. Relevant organisations such as Society of Environmental Toxicology and Chemistry (SETAC), the United States Department of Agriculture (USDA), the United States Environmental Protection Agency (USEPA), or the EU JRC (EC, 2021b) have put forward several approaches to deal with this issue (Edelen and Ingwersen, 2018; Lewandowska et al., 2021).

Most of these approaches are inspired on the **Pedigree Matrix** concept from Funtowicz and Ravetz (1990), as proposed by Weidema and Wesnæs (1996). Its adaptation to the LCA area comprises data quality attributes: reliability, temporal correlation, geographical correlation, etc. with minor differences between authors and organisations. Data quality is typically assessed on a 1-5 "semi-quantitative" (i.e. ordinal) scale on each of these attributes. As these indicators focus on inventories, Qin et al. (2020) propose a Pedigree Matrix for the impact assessment phase. Although not explicitly based on the Pedigree Matrix, EU JRC's International Reference Life Cycle Data System (ILCD) and Environmental Footprint methods also use an ordinal 1-5 scale (1«Excellent, 2«Very Good, 3«Good, 4«Fair, 5«Poor) regarding four data quality attributes.

Figure 37. Aspects for data quality considerations in SSbD.

Source: Own elaboration

The aspects illustrated in Figure 37 are recommended to be considered when assessing the data quality:

- **Technological representativeness:** SSbD assessments require data that accurately reflect the processes, technologies, and product systems under study. Technological representativeness ensures, for instance, that life cycle inventory (LCI) and exposure or hazard data correspond to the specific materials, technologies, or functions being evaluated. In SSbD, this may involve data for emerging technologies or innovative chemistries, which often necessitate proxy data and expert judgment.

- **Geographical representativeness**: Geographic relevance is key to identifying region-specific impacts and regulatory conditions. SSbD assessments should align data collection with location-specific environmental, social, and regulatory contexts, particularly where regional sourcing, emissions profiles, or occupational risks differ significantly.

- **Time-related representativeness**: Temporal relevance refers to how current the data are. SSbD calls for using recent and forward-looking data, especially in the context of innovative or pre-market materials, where prospective LCA or risk assessments may be needed.

- **Completeness**: A complete SSbD evaluation requires full coverage of the life cycle stages relevant to the material or product, including potential toxicological, ecotoxicological, and social impacts. Completeness also implies the inclusion of key emissions, resource uses, and exposure pathways across all relevant compartments (air, water, soil, human).

- **Precision/uncertainty**: SSbD decisions often face high uncertainty, particularly in early-stage assessments. The data quality assessment should explicitly consider the confidence level, variability, and documentation of underlying datasets, and include sensitivity analysis where possible. Transparent uncertainty communication is vital to ensure robust SSbD decision-making.

- **Reliability of data sources**: this aspect evaluates the trustworthiness of the data source, including its transparency, methodological soundness, and review status. Data are ranked from high to low reliability depending on whether they come from peer-reviewed publications, official statistics, expert judgments, or unverified sources. Incorporating source reliability enhances the robustness of SSbD assessments, particularly when relying on global databases with varying degrees of data transparency.

Annex 8. Reference scales and monetisation factors for the socio-economic assessment

Table 29. Reference scales examples for the socio-economic analysis.

Socio-economic aspect	Assessment method	Examples of indicators	Reference scales (examples)
Risk of child labour in the supply chain	Reference scale assessment	% of children in employment (age 7-14)	very high risk: >10 high risk: 5-10 medium risk: 2.5-5 low risk: 1-2.5 very low risk risk: <= 1
Risk of forced labour in the supply chain	Reference scale assessment	Risk of forced labour in the country (cases per 1,000 inhabitants)	very high risk: >1.2 high risk: 0.6 -1.2; medium risk: 0.4 -0.6
Fair salary	Reference scale assessment	Living wage, per month Sector average wage, per month	y, ratio Salary/Living wage 0 < y <1 very high risk 1 ≤ y < 1.5 high risk 1.5 ≤ y < 2 medium risk 2 ≤ y < 2.5 low risk 2.5 ≤ y very low risk risk
Working time	Reference scale assessment	Hours of work per employee, per week	very high risk: <20 and >60 high risk: 20 - <30 and 55 - <60 medium risk: 30 - <40 and 48 - <55 low risk: 40 - <48
Equal opportunity and discrimination	Reference scale assessment	Gender wage gap (%)	very high risk: >=30% and <=-30 high risk: 20% - <30% and -20% - >-30% medium risk: 10% - <20% and -10% - >-20% low risk: 5% - <10% and -5% - >-10% very low risk risk: 0% - <5% and 0% - >-5%
Freedom of association and collective bargaining	Reference scale assessment	Right of association (ordinal scale) Right of collective bargaining (ordinal scale) Right to strike (ordinal scale)	very high risk: 0 high risk: 1 low risk: 2 very low risk risk: 3
		Trade union density (% of employees organized in trade unions)	very high risk: 0-20% high risk: >20-40% medium risk: >40-60% low risk: >60-80% very low risk risk: >80%
Presence of safety measures	Reference scale assessment	Preventive measures and emergency protocols exist regarding pesticide and chemical exposure Adequate general occupational safety measures	Qualitative reference scale to be developed by the practitioner based on - the management practices and strategies the organisation guarantees in terms of health and safety of its own workers and in its community of suppliers. - the maintenance and promotion of workers' health and working capacity; - the improvement of working environment and work to become conducive to safety and health and development of work organisations and working cultures in a direction which supports health and safety at work - the status of prevention measures and management practices; the extent to which the management maintains or improves the safety and overall health status of the workers. (E.g. investments in prevention measures, trainings, procedure in place to collect complaints regarding its own workers; investments in partnerships that improve the health and safety in the region the company purchases from).

		Preventive measures and emergency protocols exist regarding accidents and injuries (cases of violation per 100,000 employees)	very high risk:> 0.0565 high risk: 0.0215 - < 0.0565 medium risk: 0.0095- < 0.0215 low risk: 0.0025 - < 0.0095 very low risk risk: < 0.0025
Accidents at work	Reference scale assessment	Rate of non-fatal accidents at workplace (cases per 100.000 employees and year)	very high risk: ≥ 3000 high risk:2250 – 3000 medium risk: 1500 – 2250 low risk: 750 – 1500 very low risk risk: 0 – 750
		Rate of fatal accidents at workplace (cases per 100.000 employees and year)	very high risk: ≥ 40 high risk: 25 -40 medium risk: 15-25 low risk: 7.5 -15 very low risk risk: 0 -7.5
Safe and healthy living conditions	Reference scale assessment	Organisation efforts to strengthen community health (e.g. high risk through shared community access to organisation health resources) Management effort to minimize use of hazardous Substances Management oversight of structural integrity	Qualitative reference scale to be developed by the practitioner based on: - The extent to which the company or facility works to prevent and mitigate adverse impacts or enhance positive impacts on the health and safety of the local community - Evidence that the company invests and have procedure in place to communicate potential health and safety impacts of their operations to surrounding communities. - Institution of environmental risk management systems for preventing, mitigating and controlling health damage from operations.
Contribution to GDP	Reference scale assessment	Contribution of the product/service/organisation to economic progress (e.g. annual growth rate of real GDP per employed person; sector level: % of GPD)	no opportunity: 0-<1 low opportunity: 1-10 medium opportunity: >10-25 high opportunity: >25
Creation of knowledge-intensive employment	Reference scale assessment	Knowledge intensive jobs (% high-skilled employees (ISCO level 3-4) /total employees required for a unit of production)	< 20% No opportunity/risk opportunity 20% – 39% Low opportunity 40% – 59% Moderate opportunity ≥ 60% High opportunity
Supply chain vulnerabilities	Identification of CRM	N° of flags related to the presence of CRM as material inputs, based on EC methodology. Total mass of CRMs; to be complemented with additional qualitative assessment of supply chain vulnerability.	Reference scale to be developed by the practitioner based on the number of flags for CRM and additional considerations on supply chain vulnerabilities-
Technology potential	Reference scale assessment	Patent growth rate in % of this technology for a defined period (e.g. 5 years).	≥ 20% High opportunity (High innovation potential) 5% – 19% Moderate opportunity 0% – 4%Moderate risk < 0% (decline) High risk
Skill shortages risk	Reference scale assessment	Ratio of training investment per employee vs. industry benchmarks.	Ratio (Company / Industry Benchmark) ≥ 1.2 Low risk / Positive contribution 0.8 – 1.19 Moderate risk 0.5 – 0.79 Elevated risk < 0.5High risk
Life cycle costs	Life Cycle Costing, including societal costs	Internal costs (incl. e.g. material acquisition, labour, energy, etc) Externalities (through risk monetisation of environmental impacts)	Not applicable. Comparative assessment between options

Sources: Loubert et al. 2023; Orienting Del. 2.5c; authors elaboration

Table 30. Set of monetary valuation coefficients as proposed in Gama Caldas et al. (2024).

Impact category		**Unit of measure**	**Value**
1	Climate change, total	€$_{2019}$/kg CO_2 eq.	$1.00x10^{-1}$
2	Ozone depletion	€$_{2019}$/kg CFC-11 eq.	$5.55x10^{+1}$
3	Human toxicity, cancer	€$_{2019}$/CTUh	$1.66x10^{+5}$
4	Human toxicity, non-cancer	€$_{2019}$/CTUh	$9.19x10^{+5}$
5	Particulate matter	€$_{2019}$/disease incidence	$7.28x10^{+5}$
6	Ionising radiation, human health	€$_{2019}$/kBq U_{235} eq.	-
7	Photochemical ozone formation, human health	€$_{2019}$/kg NMVOC eq.	$1.20x10^{0}$
8	Acidification	€$_{2019}$/mol H^+ eq.	$3.50x10^{-1}$
9	Eutrophication, terrestrial	€$_{2019}$/mol N eq.	-
10	Eutrophication, freshwater	€$_{2019}$/kg P eq.	$1.95x10^{0}$
11	Eutrophication, marine	€$_{2019}$/kg N eq.	$3.27x10^{0}$
12	Ecotoxicity, freshwater	€$_{2019}$/CTUe	$3.89x10^{-5}$
13	Land use	€$_{2019}$/pt	$1.78x10^{-4}$
14	Water use	€$_{2019}$/m^3 water eq. of deprived water	$5.08x10^{-3}$
15	Resource use, minerals, and metals	€$_{2019}$/kg Sb eq.	-
16	Resource use, fossils	€$_{2019}$/MJ	-

Source: Own elaboration

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