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Safe and Sustainable by Design chemicals and materials

Framework for the definition of criteria and evaluation procedure for chemicals and materials

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Authors' contribution

Carla Caldeira contributed to the concept, development of the whole framework and development of Step 3 and 4 of the framework, **Lucian R. Farcal** contributed to the concept, the development of Step 1 and 2 of the framework and Section 6 of the report, **Irantzu Garmendia** contributed to the development of Step 2 and 3 of the framework and reviewed the overall framework, **Lucia Mancini** developed Step 5 of the framework and reviewed the report, **Davide Tosches** and **Antonio Amelio** contributed to the development of Section 4.1 and Section 6.1 and supported the editing process, **Kirsten Rasmussen**, **Hubert Rauscher** and **Juan Riego Sintes** contributed to the concept, and reviewed the overall framework, **Serenella Sala** is the project responsible at the JRC. She contributed to the concept and development of the whole framework.

Executive summary

Context

Within the European Green Deal, the Chemicals Strategy for Sustainability (CSS) (EC, 2020a) identified a number of actions to reduce negative impacts on human health and the environment associated with chemicals, materials, products and services commercialised or introduced onto the EU market. In particular, the ambition of the CSS is to phase out the most harmful substances and substitute, as far as possible, all other substances of concern, and otherwise minimise their use and track them. This objective requires novel approaches to analysing and comparing, across all life cycle stages, effects, releases and emissions for specific chemicals, materials, products and services, and move towards zero-pollution for air, water, soil and biota.

The **European Union (EU) CSS action plan** foresees the **development of a framework to define safe and sustainable by design (SSbD) criteria for chemicals and materials** that should contribute to achieve the Green Deal ambitions, going beyond current regulatory compliance. This **report aims at proposing such a framework**, presenting the dimensions, aspects, methods, and indicators that can be used to assess chemicals and materials and how criteria can be defined in order to identify those that are SSbD.

The aim of the SSbD framework is to **support the design and development of safe and sustainable chemicals and materials with research and innovation (R&I) activities**. The **SSbD framework will be tested**, via the execution of case studies that will support the refinement of the framework and criteria. This phase will aim to **identify and collect bottlenecks, and measures to address them will be explored. Research outputs** generated by implementing the SSbD framework and criteria **will feed into relevant EU policies/initiatives.**

The information presented in this report is the wider **scientific and technical input for the European Commission's work on developing recommendations for Safe and Sustainable by Design,** which might not necessarily include all elements herein presented.

Objectives of the framework

The **application of the SSbD framework aims at**:

- Promoting the application of the Safe and Sustainable by Design approach to chemicals and materials and steering innovation towards the green industrial transition, resulting in the EU becoming a global reference for safety and sustainability targets;
- Providing guidance on criteria development for the design of 'safe' and 'sustainable' chemicals/materials;
- Driving innovation towards the substitution or minimisation of the production and use of substances of concern, in line with and beyond upcoming regulatory obligations;
- Minimising or, as far as possilbe, eliminating the impact on human health, climate and the environment (air, water, soil) along the entire chemical's and material's life cycle;
- Enabling comparative assessment of chemicals and materials based on safety and sustainability performance for a given function or application context.

Definitions (presented in Annex 1)

When applied in the context of chemicals/materials, the concept of **sustainability** could be formulated as the **ability of a chemical/material[1] to deliver its function without exceeding environmental and ecological boundaries along its entire life cycle, while providing welfare, socio-economic benefits and reducing externalities.**

The **safety** concept is transversal to all sustainability dimensions (environmental, social and economic) and it is related to the **absence of unacceptable risk** (in line with REACH art 68 (EU, 2006)) **for humans and the**

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[1] This definition also applies to products and services.

environment, preferably ensured by avoiding chemicals and materials with intrinsic hazard properties.

Principles underpinning the framework

A set of principles were defined underpinning the development of the new framework and that are essential for its (future) operationalisation:

- Define a hierarchy between safety and other sustainability dimensions to avoid regrettable substitution;
- Move from relative (safer and more sustainable) to absolute[2] (safe and sustainable) improvements ensuring that chemicals and materials are produced and used without exceeding acceptable boundaries;
- Define cut-off criteria for the design of chemicals and materials to stimulate sustainable research & innovation, based on data beyond the current regulatory information requirements;
- Establish close links to ‘functionality oriented’ research on alternatives development;
- Focus on continuously and iteratively minimising environmental pressures, using dynamic boundaries and cut-offs, so that the framework may become a tool of management of improvements along the innovation trajectory. This enables a process of continuous improvement (contrary to static one-time improvement);
- Optimal use of the full data-space on adverse effects. For every (new) chemical/material a similarity comparison should be made with the full spectrum of structurally or functionally similar substances to assess the expected potential to cause negative impact. According to the precautionary principle, each indication of a potential adverse effects should stimulate further assessment. This should serve as a basis for further action;
- Communicate SSbD actions taken, including data, throughout the supply chain (including yearly reports); make all data available in FAIR (findable, accessible, interoperable and reusable) format, to enhance also the transparency, accountability and duty of care;
- Promote the use of a coherent framework across different policies such as REACH, Sustainable Finance, Sustainable Products Initiative (SPI) and others.

Framework features

The proposed SSbD framework to assess chemicals and materials follows a **hierarchical approach** in which safety aspects are considered first, followed by environmental, social and economic aspects. The last two are included in the framework to be explored as methods still need to be further developed.

The SSbD framework proposed is a **general approach for the definition of criteria for SSbD for chemicals and materials**. It is broadly applicable allowing the definition of a set of operational criteria that can be implemented and that increase or ensure compliance with reference targets for safety and sustainability of chemicals and materials. It **can be applied to newly developed chemicals and materials or to existing ones**. For the latter, the framework can be used i) to **support the redesign of their production processes** by evaluating alternative processes to improve their safety and sustainability performance, or ii) to **compare them on the basis of SSbD** criteria (e.g. for innovation by substitution with better performing chemicals/materials, in terms of safety and sustainability, or selection in downstream application).

The framework foresees the assessment of the **entire life cycle of a chemical or material**, including the design phase and considering among others its **functionality and end-use(s)**. Therefore, even if the

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[2] The term absolute sustainability refers to the possibility of a chemical to comply with safety and to carry limited environmental impacts, namely within planetary boundaries. Moving from comparative consideration (A better than B) to absolute considerations (A is absolutely sustainable) requires to include elements of the use (which use and how much) which goes beyond what is currently proposed in the framework. However, several elements of the framework are enabling consideration which are going beyond the mere comparison of chemicals and are moving the assessment towards more boundary oriented assessment.

evaluation of products is outside the scope of this framework, the use of the chemicals/materials in products is considered.

Framework structure: a stepwise approach

The SSbD framework entails **two components**:

1. a **(re)design phase** in which design guiding principles are proposed to support the design of chemicals and materials, and
2. a **safety and sustainability assessment** phase in which the safety, environmental and socio-economic sustainability of the chemical/ material is assessed.

The **safety and sustainability assessment** herein presented allows the identification of SSbD chemicals and materials, in particular how criteria can be defined. It comprises **5 Steps** that can be carried out sequentially or in parallel, depending on the data and tools availability and the specific purpose of the exercise. Moreover, the assessment can be done and, in many cases, should be done iteratively to optimise the results. The steps are:

Step 1 – Hazard assessment of the chemical/material

The first step looks at the intrinsic properties of the chemical or material in order to understand their hazard potential before further assessing the safety during use.

Step 2 – Human health and safety aspects in the chemical/material production and processing phase

In this step, the health and safety aspects related to the chemical/material production and processing are assessed. It covers all processes from the raw material extraction (from natural resources) to production (e.g. substance manufacturing), processing (e.g. mixing), recycling or waste management. And addresses occupational safety and health (OSH) related aspects in each of them.

Step 3 – Human health and environmental aspects in the final application phase

This step assesses the application/use-specific exposure to the chemical/material and the associated risks, both for human health and the environment.

Step 4 – Environmental sustainability assessment

The fourth step considers impacts along the entire chemical/ material life cycle by means of Life Cycle Assessment, assessing several environmental impact categories such as climate change and resource use.

Step 5 – Social and economic sustainability assessment

The fifth step relates to Social and Economic Sustainability assessment, to provide information on the scientific basis and available approaches for the assessment of socio-economic impacts. Given the limited level of implementation and methodological maturity this step is in an exploratory phase.

Evaluation

The evaluation of the chemical/materials will be performed considering:

1. The adherence to the SSbD principles;
2. The sustainability assessment, namely the detailed figures on the performance of the chemical/material against the SSbD criteria.

A dashboard summarising the results of the sustainability assessment is proposed as a tool to facilitate informed conclusions/decisions based on a holistic assessment. The result of the evaluation can be expressed either as **a class of SSbD** (poor, good, very good) or with a **numerical score** derived from the combination of the individual scores of each aspect (subject to e.g. weighting). The **evaluation procedure shall take into account the lack of data and data uncertainty** inherent to the assessment.

Abstract

Within the European Green Deal, the Chemicals Strategy for Sustainability (CSS) (EC, 2020b) identified a number of actions to reduce negative impacts on human health and the environment associated with chemicals, materials, products and services commercialised or introduced onto EU market. The EU CSS foresees the development of a framework to define Safe and Sustainable by Design (SSbD) criteria for chemicals and materials that should contribute to achieve the Green Deal ambitions.

This report presents a framework to develop criteria for chemicals and materials in the context of the EU CSS. It presents the dimensions, aspects, methods and indicators that can be used to assess chemicals and materials and how criteria can be defined in order to identify those chemicals and materials that are SSbD. An evaluation procedure is proposed to rank chemicals and materials to identify 'best in class' on sustainability performance and those that call for improvements or even need to be substituted or phased out.

The SSbD framework entails a (re)design phase in which design guiding principles are proposed to support the design of chemicals and materials, and a safety and sustainability assessment phase in which the safety, environmental and socio-economic sustainability of the chemical/ material is assessed. The overall safety and sustainability assessment comprises five steps. The first three steps assess safety aspects such as the hazard properties (Step 1), the human health and safety aspects in the chemical/material production and processing phase (Step 2), and the human health and environmental effects in the final application phase (Step 3). Further, Step 4 assesses impacts along the entire chemical/ material life cycle, and Step 5 explores socio-economic aspects, focusing on the available approaches and suggesting potential streamlined assessment methods. The present report is focused on the definition of criteria for assessing chemicals/materials for safety and environmental sustainability.

The aim of the SSbD framework is to support the design and development of safe and sustainable chemicals and materials within the research and innovation (R&I) phase. The SSbD framework will be tested, via the execution of case studies that will support the refinement of the framework and criteria. This phase will aim to identify and collect bottlenecks, and measures to address them will be explored. Research outputs generated by implementing the SSbD framework and criteria will feed into relevant EU policies/initiatives.

The information presented in this report is the wider scientific and technical input to the European Commission's work on developing recommendations for Safe and Sustainable by Design, which might not necessarily include all elements herein presented.

1. Introduction

The European Green Deal is one of the priorities of the European Commission (EC), which aims to transform the EU's current economy into a greener and more sustainable one (EC, 2019a). Within the Green Deal, the Chemicals Strategy for Sustainability (CSS) (EC, 2020a) identified a number of actions intended to reduce negative impacts on human health and the environment associated with chemicals, materials, products and services commercialised or introduced onto the EU market. In particular, the ambition of the CSS is to phase out the most harmful substances (unless they are proven to be essential for the society and there are no safer alternatives) and substitute, as far as possible, all other substances of concern (*defined in Article 2(28) of the Sustainable Products Initiative (SPI) proposal* (EC, 2021b; EC, 2022a)), and otherwise minimise their use and track them. This objective requires novel approaches to analysing and comparing, across all life cycle stages, effects, releases and emissions for specific chemicals, materials, products and services, moving towards zero-pollution for air, water, soil and biota.

The EU CSS action plan **foresees the development of a framework to define safe and sustainable by design** (SSbD) criteria for chemicals and materials that should contribute to achieve the Green Deal ambitions, beyond current regulatory compliance. The SSbD is an approach to support the design, development, production, and use of chemicals and materials that focuses on providing a desirable function (or service), while avoiding or minimising negative impacts to human health and the environment. The SSbD concept integrates aspects from the domain of safety, circularity and functionality of chemicals and materials with sustainability considerations throughout their entire lifecycle, in order to minimise their environmental footprint. SSbD aims at facilitating the industrial transition towards a safe, zero pollution, climate-neutral and resource-efficient production and consumption, addressing adverse effects on humans, ecosystems and biodiversity from a lifecycle perspective (EC, 2020a).

*At this stage, **safe and sustainable by design can be defined** as a pre-market approach to chemicals and materials design that focuses on providing a function (or service), while **avoiding volumes and chemical and material properties that may be harmful to human health or the environment, in particular groups of chemicals likely to be (eco)toxic, persistent, bio-accumulative or mobile.** Overall sustainability should be ensured by minimising the environmental footprint of chemicals and materials in particular in relation to **climate change, resource use, and protecting ecosystems and biodiversity, adopting a lifecycle perspective** (adapted from* EC (2020a)).

Hence, the SSbD approach targeted by the CSS goes beyond traditional green chemistry innovation approaches by integrating life cycle and safety aspects into the design phase of systems and processes for the production and use of chemicals and materials. Such an approach would augment tangible benefits for society and the environment in the global value chain, avoiding unintended shifts of impacts on human and environmental health. To fulfil these ambitions, there is the need to develop a new framework for the definition of safe and sustainable by design criteria for chemicals and materials (Gottardo et al., 2021).

The application of the SSbD framework aims at:

- **Promoting the application of the Safe and Sustainable by Design approach to chemicals and materials and steering innovation towards the green industrial transition**, outlining which and how safety and sustainability should be considered in the design phase and innovation process of chemicals and materials, resulting in the EU becoming a global reference for safety and sustainability targets. Applying SSbD criteria in the research and innovation phase of chemicals and materials will help industry to prioritise innovation according to policy priorities and future developments. Morevover, it will minimise undesired environmental and health impacts and increase beneficial ones. This will reduce substantial and expensive modifications in later phases of the development process, as it is more effective to integrate such aspects in early stages of the design phase. This aim is closely linked to policy priorities related to Industrial Strategy, Green Deal and Sustainable finance.[3]

- **Providing guidance on how to develop criteria for the design of 'safe' and 'sustainable' chemicals and materials** and how to assess them against those criteria.
- **Driving innovation towards the substitution or minimisation of the production and use of substances of concern**, in line with and beyond upcoming regulatory obligations. The use of SSbD criteria will help avoiding regrettable substitutions (i.e. solving one problem and creating others) and ensure the availability of consistent, transparent and updated information on properties and uses of chemicals and materials across the value chain (in support to other Commission policies like Sustainable Products Initiative, REACH revision, revision of product specific legislation and the zero pollution ambition).
- **Minimising or, as far as possilbe, eliminating the impact on human health, climate and the environment** (air, water, soil) along the chemical's and material's entire life cycle, ensuring sustainable circularity (aligned with Circular Economy Action Plan, Climate neutrality, Zero Pollution Action Plan, Farm to Fork Strategy, Bioeconomy Strategy). Chemicals release during the life cycle is also considered.
- **Enabling comparative assessment of chemicals and materials based on safety and sustainability performance** for a given function or application context.

The aim of the SSbD framework is to **support the design and development of safe and sustainable chemicals and materials within the research and innovation (R&I) phase**. The **SSbD framework will be tested**, via the execution of case studies that will support the refinement of the framework and criteria. For the testing and demonstration of the SSbD framework, data generated using **new approach methodologies (NAMs)** should be prioritised and included as much as possible in the case studies, while fulfilling the data quality criteria as well as the **principles on findable, accessible, interoperable and reusable (FAIR) data**.

This phase will aim to **identify and collect bottlenecks, and measures to address them will be explored. Research outputs** generated by implementing the SSbD framework and criteria **will feed into relevant EU policies/initiatives.**

The information presented in this report is the **wider scientific and technical input** for the European Commission's work on **developing recommendations for Safe and Sustainable by Design**, which might not necessarily include all elements herein presented here.

Figure 1 illustrates the approach taken for the development of the SSbD framework. The first step was a review of existing frameworks for SSbD and related concepts, which aimed at identifying what safety and sustainability dimensions are included in existing frameworks as well as the methods, models, tools, and indicators used to address the key issues at stake. Several frameworks were reviewed including initiatives from research, industry, governmental agencies and NGOs (Caldeira et al., 2022).

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[3] The SSbD framework should be harmonised, as far as possible, with other relevant initiatives that are implemented or are being developed such as the EU Ecolabel (EU, 2010), the EU Green Public Procurement (EC, 2021b), the Ecodesign requirements for energy-related products (EU, 2009), the framework for energy labelling (EU, 2017), and the Sustainable Products Initiative (EC, 2021c; EC, 2022b) and the related proposal for a regulation for establishing a framework for setting ecodesign requirements for sustainable products (EC, 2022a). Regarding the latter, it is recognised that the actions translated in the EU Action Plan Towards zero pollution for air, water and soil and the Chemicals Strategy for Sustainability, imply that chemicals, materials and products have to be as safe and sustainable as possible by design and during their life cycle, leading to non-toxic material cycles. It is important to consider as well other actions being developed in the context of CSS such as: development of an indicator framework (i.e. Key Performance Indicators action) to measure the industrial transition towards the production of safe and sustainable chemicals, REACH and CLP as revised, establishing i.e. essential use, one substance one assessment approach and substitution of substances of concern, and policy commitments to phase out most harmful substances in consumer products and professional uses, and to minimise production and use of substances of concern. Moreover, other EU initiatives such as the EU Sustainable Finance (Platform on Sustainable Finance., 2021), including the EU taxonomy for sustainable activities, are also relevant in the context of SSbD.

Figure 1. Overview of the SSbD framework development process

Building on the learnings from the review and considering the aims of the framework, a set of principles was defined underpinning the development of the new framework:

- Define a hierarchy between safety and other sustainability dimensions to avoid regrettable substitution;
- Move from relative (safer and more sustainable) to absolute[4] (safe and sustainable) improvements ensuring that chemicals and materials are produced and used without exceeding acceptable boundaries;
- Define cut-off criteria for the design of chemicals and materials to stimulate sustainable research & innovation, based on data beyond the current regulatory information requirements;
- Establish close links to 'functionality oriented' research on alternatives development;
- Focus on continuously and iteratively minimising environmental pressures, using dynamic boundaries and cut-offs, so that the framework may become a tool of management of improvements along the innovation trajectory. This enables a process of continuous improvement (contrary to static one-time improvement);
- Optimal use of the full data-space on adverse effects. For every (new) chemical/material a similarity comparison should be made with the full spectrum of structurally or functionally similar substances to assess the expected potential to cause negative impact. According to the precautionary principle, each indication of a potential adverse effects should stimulate further assessment. This should serve as a basis for further action;
- Communicate SSbD actions taken, including data, throughout the supply chain (including yearly reports); make all data available in FAIR (findable, accessible, interoperable and reusable) format, to enhance also the transparency, accountability and duty of care;

- Promote the use of a coherent framework across different policies such as REACH, Sustainable Finance, Sustainable Products Initiative (SPI) and others.

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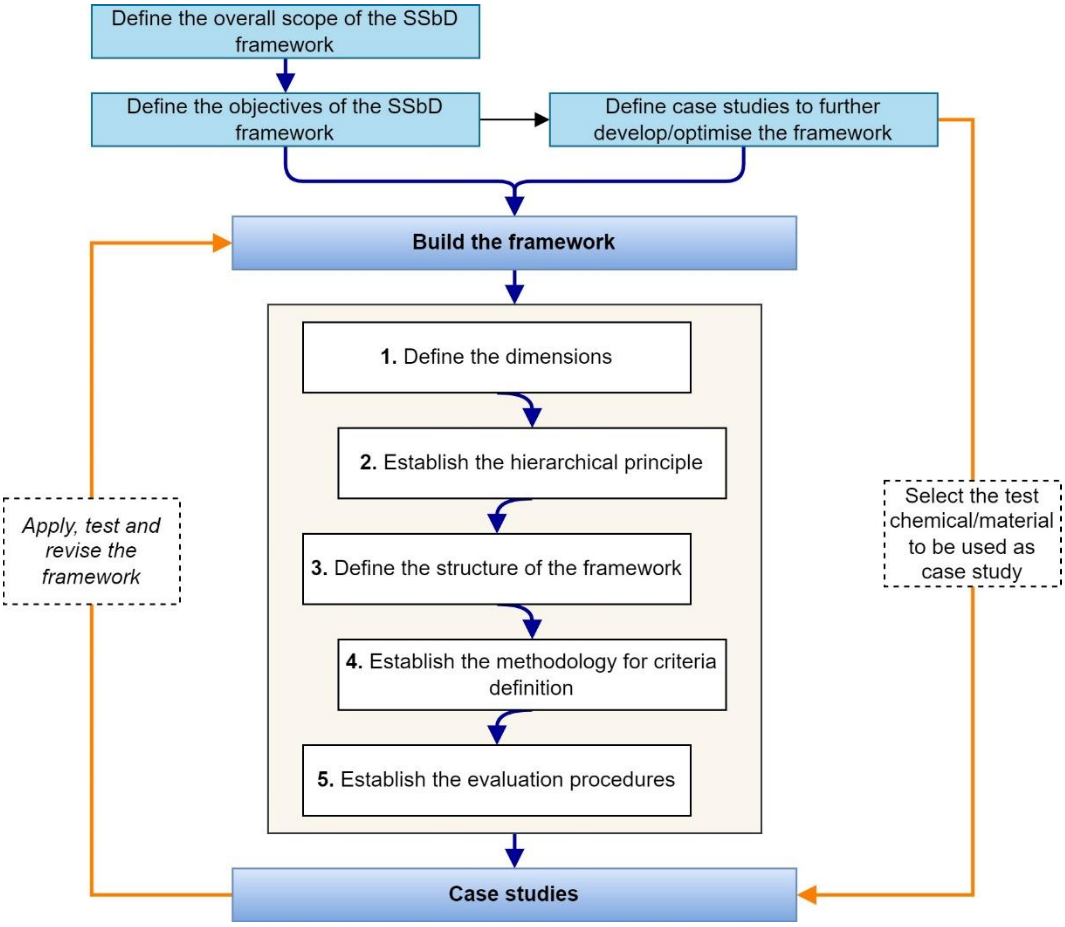
[4] The term "absolute sustainability" refers to the possibility of a chemical to comply with safety and to carry limited environmental impacts, namely within planetary boundaries. Moving from comparative consideration (A better than B) to absolute considerations (A is absolutely sustainable) requires to include elements of the use (which use and how much) which goes beyond what is currently proposed in the framework. However, several elements of the framework are enabling consideration which are going beyond the mere comparison of chemicals and are moving the assessment towards more boundary oriented assessment.

Considering the above, a new framework was developed - including a methodology for the definition of possible SSbD criteria and implementation mechanisms- following the iterative process reported in (Figure 2). After the initial scoping phase, the framework has been built via:

1. Defining the assessment dimensions to be considered in the SSbD framework;
2. Establishing the hierarchical principle underpinning the SSbD framework;
3. Defining the structure of the framework and the aspects to be included in each assessment step;
4. Establishing the methodology for criteria definition;
5. Establishing the procedures for evaluating the criteria (e.g. scoring system, levels).

These steps will then be tested and refined within the dedicated case studies in the next phase of the project.

Figure 2. Overview of the iterative process established for the SSbD framework development



This report contains six additional sections. **Section 2** covers the basic concepts underpinning the framework; **Section 3** presents the building blocks of the proposed framework, including definitions and dimensions covered; **Section 4** describes the structure of the framework and the steps envisaged; **Section 5** covers the evaluation procedure; **Section 6** addresses data availability and quality; finally, **Section 7** provides some concluding remarks.

2. Background concepts underpinning the SSbD framework

The Safe and Sustainable by Design framework builds on different underpinning concepts and approaches as illustrated in Figure 3 and described in the following sub-sections.

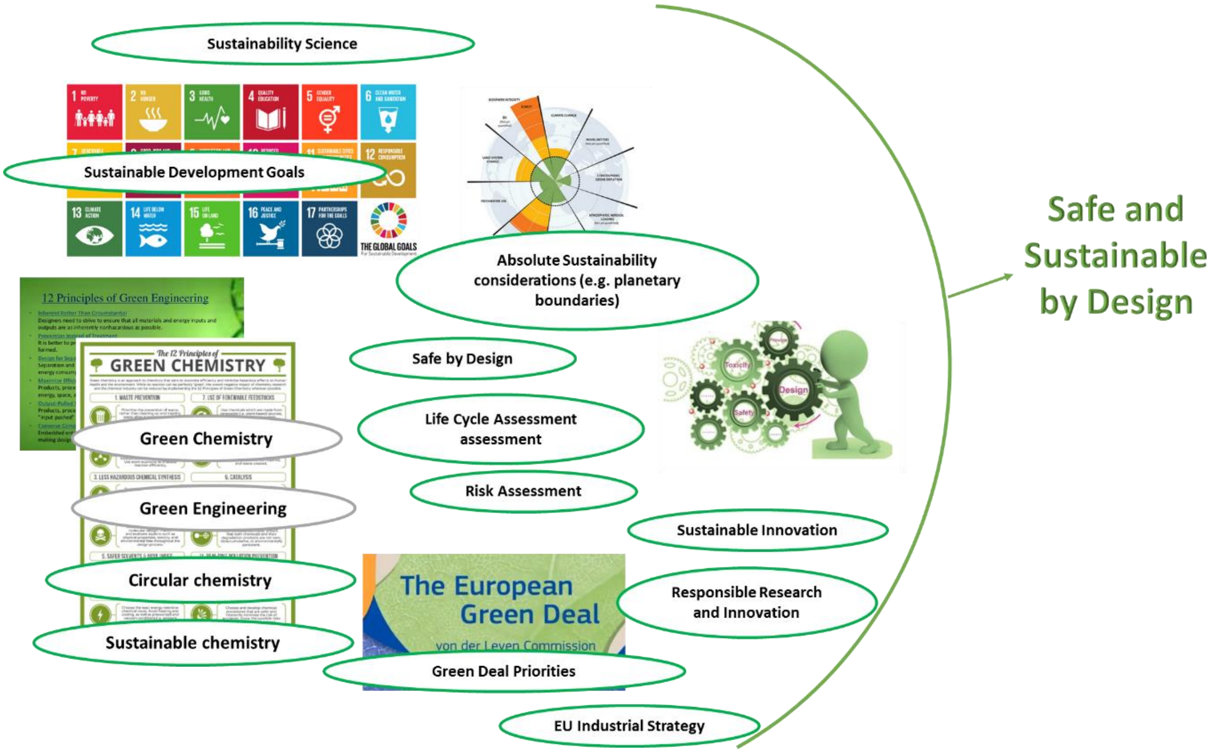


Figure 3. Underpinning principles and approaches informing the Safe and Sustainable by Design framework

2.1 Sustainability, safety, and sustainable development goals

The idea that economic growth could be compatible with environmental limits and social fairness and justice led to the concept of **sustainable development**, defined in the Brundtland Report of the World Commission on Environment and Development, Our Common Future, as the humanity's ability of meeting *"the needs of the present generations without compromising the ability of future generations to meet their own needs*" (WCED, 1987). While this definition leaves space for different interpretations, it was pivotal in shaping the most common representation of the sustainability concept, i.e. the composition and interactions between three pillars: economy, environment and society. This definition also underpins the definition of sustainability considered in the ISO Guide 82:2019 providing guidelines for addressing sustainability in standards where "*sustainability refers to a state of the global system, encompassing the environmental, social and economic subsystems, in which the needs of the present are met without compromising the ability of future generations to meet their needs*." (ISO, 2019).

The ability of current and future generation to meet their needs is associated to a development which remains within the limit of the planet. Indeed, the need to operate within a safe space respecting Earth's ecological limits was translated into the so-called **Planetary Boundaries** (PB) framework developed by (Rockström et al., 2009a, b). This framework defines the preconditions for sustainable development by identifying and quantifying environmental planetary boundaries that must not be transgressed by human activities thus avoiding unacceptable environmental change. Assessing a system in term of contribution to transgressing planetary boundaries, means to perform an **Absolute Environmental Sustainability[5] Assessment**. The PB framework

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[5] The term "absolute environmental sustainability" refers to the possibility of a chemical to comply with safety while limiting the environmental impacts, kept within planetary boundaries. Moving from comparative consideration (A better than B) to absolute considerations (A is absolutely sustainable) requires to include elements of the chemical use (which use

defines nine planetary boundaries: Climate Change, Biosphere Integrity, Stratospheric Ozone Depletion, Ocean Acidification, Biochemical Flows, Land-system change, Freshwater use, Atmospheric aerosol loading, and Novel Entities (previously called 'chemical pollution' (Rockström et al., 2009b). From these PB, Functional diversity (as part of Biosphere integrity), and Atmospheric aerosol loading are not yet quantified as per the 2015 PB update (Steffen et al. 2015). . However, in a recent publication by Persson et al. (2022), the authors 'submit that the safe operating space of the PB of Novel Entities is exceeded since annual production and releases of a continuously increasing number and amount of chemicals and other novel entities are increasing at a pace that outstrips the global capacity for assessment and monitoring', including the management of risks, which emphasises the urgency in transforming the chemical economy beyond relative improvements. Another critical point identified by the authors is the diversity of chemical entities which requires the development of a flexible SSbD framework. On this point, Fenner and Scheringer (2021), advocate for a "chemical simplification", in which, in agreement with Kümmerer et al. (2020), the number of chemicals used in many products, in particular in consumer products, needs to be reduced. This would minimise human and environmental exposure on a large scale and contribute to the achievement of a circular economy as materials that are designed for recycling need to be chemically simple.

Recently, the boundary on the freshwater has been updated, flagging another critical overcoming of sustainability threshold (Wang-Erlandsson et al, 2022). It should be noted however that at present there is limited knowledge about where these boundaries lie, in particular with respect to the production and release of man-made chemicals.

Besides the environmental, social and economic considerations, the integration of additional pillars related to institutional, cultural, and technological issues has also been proposed (e.g. (O'Connor, 2006; Vos, 2007). Partnership and peace were recognised as critical components of sustainability (UN, 2015). Furthermore, awareness of the interplay between all the sustainability pillars and related goals and targets has increased.

Hence, the concept of sustainability has evolved over time, leading to the development of the so-called **sustainability science**[6] which is translating sustainability principles into practical solutions. The concern about the use of natural resources in relation to the population growth dates back to the 18th century, when political economists such as Thomas Robert Malthus drew attention to the use of natural resources in this context (Purvis et al., 2019). The modern concept of sustainability originated in the 1970s, being popularly attributed to the Club of Rome's report "Limits to Growth" (Meadows et al., 1972). One of the arguments of the popular essay was that the modern growth-based economy was unsustainable on a finite planet. It is interesting to note that around 1967, the safety of chemicals was addressed at the EU level by the agreement of the Dangerous Substances Directive (Directive 67/548/EEC). Since then, chemicals legislation has evolved and expanded significantly, based on a deeper understanding of effects of chemicals on human health and the environment.

The sustainability principles have been enunciated in terms of specific goals for humankind, the United Nations' **Sustainable Development Goals** (SDGs). The 17 SDGs, including 169 targets and 231 indicators, are defined in the Agenda 2030 (UN, 2015) and set out a vision for a future global society. The 2030 Agenda for Sustainable Development covers the different dimensions of sustainability, providing principles and reference for policy at different levels (local, national and regional level) and for business and corporate decision makers. The European Union has committed to play a pivotal role in SDGs achievements (EC, 2016) and to align its development policy with the SDGs (EC, 2019b). In recent years, the academic and political community is moving away from the "triple bottom line" model for sustainability towards models, where economics (as an arbitrary, human-introduced feature) receives less importance, and where the societal domain (which encapsulates economic

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and how much) which goes beyond what currently proposed in the framework. However, several elements of the framework are enabling consideration which are going beyond the mere comparison of chemicals and are moving the assessment towards more boundary oriented assessment.

[6] A solution-oriented discipline that studies the complex relationship between nature and humankind, conciliating the scientific and social reference paradigms which are mutually influenced- and covering multi temporal and spatial scales. The discipline implies a holistic approach, able to capitalize and integrate sectorial knowledge as well as a variety of epistemic and normative stances and methodologies towards solutions' definition' (Sala et al. 2013a)

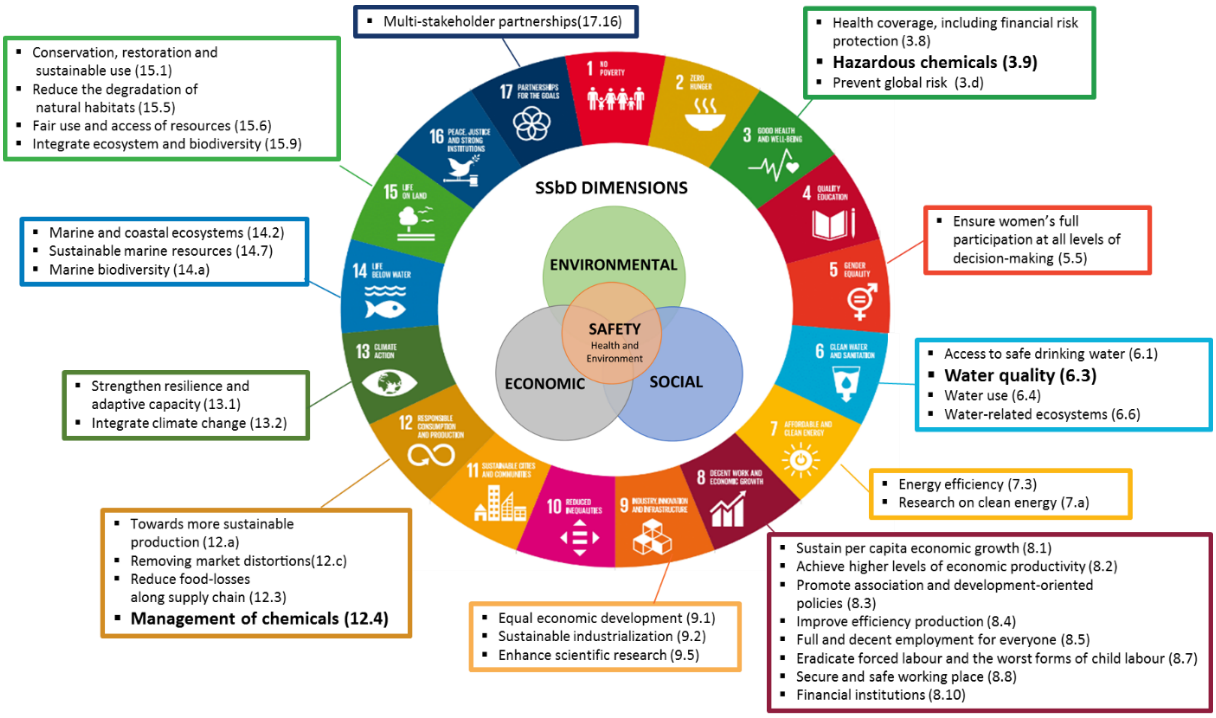
markets) is itself embedded in the wider, more overarching environmental domain of sustainability as illustrated in the "doughnut model") (Raworth 2017 ; Rockström, 2015).

The transition towards SSbD chemicals and materials will contribute to several SDGs as depicted in Figure 4. In particular, SDG 3 Good Health and Wellbeing Target 3.9 'By 2030, substantially reduce the number of deaths and illnesses from hazardous chemicals and air, water and soil pollution and contamination', SDG 12 Sustainable Consumption and Production Target 12.4 'By 2020, achieve the environmentally sound management of chemicals and all wastes throughout their life cycle, in accordance with agreed international frameworks, and significantly reduce their release to air, water and soil in order to minimise their adverse impacts on human health and the environment', and SDG 6 Water Quality Target 6.3 'By 2030, improve water quality by reducing pollution, eliminating dumping and minimising release of hazardous chemicals and materials, halving the proportion of untreated wastewater and substantially increasing recycling and safe reuse globally' (UN, 2015).

The SSbD concept literally emphasises **safety and sustainability**, nevertheless this distinction in not crystal clear as **safety is an inherent element of both environmental (pollution) and social (health) aspects of sustainability, and it has an economic component as well.** In the regulatory context, "Safety" is defined based on thresholds for human or environmental impacts. Indeed, the challenge is to understand (and define metrics and criteria for) how thresholds for "Safety" can or should be aligned with physically derived targets or limits for impacts on human health and environment, which is the prevailing concept in the "Environment" dimension.

While recognising that safety is an integral part of the three sustainability dimensions, in this report we specifically address the safety component and therefore this is reflected as the four dimensions underpinning the SSbD, as illustrated in Figure 4. This helps in mapping the different aspects that are covered to ensure a comprehensive SSbD assessment.

Figure 4. Dimensions considered in the SSbD and related SDGs targets



In the sustainability science debate, there are proposals to present the SDGs giving emphasis to the role of environment and ecosystems as building blocks for socio-economic development (Figure 5). This is in line with the so-called "strong sustainability" approach, where the conservation of the natural capital is the main objective and where the increase in economic and social capital should not happen at the expense of natural capital.

Figure 5. A presentation of the economy and society related SDGs as dependent upon the biosphere and its integrity (credit: Azote Images for Stockholm Resilience Centre)

2.2 Green chemistry, sustainable chemistry, circular chemistry, green engineering, safe by design

To design a safe and environmentally sustainable chemical/material, several principles have been proposed over time. The proposed principles are those considered e.g. in **green chemistry** (Anastas and Warner, 1998) **green engineering** (Anastas and Zimmerman, 2003), **sustainable chemistry** (Blum et al. 2017; ISC3, 2021; UBA, 2009; UNEP, 2021a), **circular chemistry** (Keijer et al. 2019) and **safe by design** (OECD, 2020) (a list is available in Annex 2) as well as policy related ambitions (e.g. transition to a circular economy (EC, 2020b) to a bioeconomy (EC, 2018a); to zero pollution (EC, 2021d). Many of these principles includes both safety and resources related considerations and intend to help the design or redesign of chemicals, materials and their related manufacturing processes and supply-chains.

With regards to safety, the **safe by design** (SbD) concept is integrating safety in the design process (Dekkers et al., 2020; OECD, 2020; Jantunen et al., 2021; Tavernaro et al., 2021). In the context of Safe Innovation Approach (SIA), developed specifically for nanomaterials (Soeteman-Hernandez et al., 2019; OECD, 2020), SbD refers to identifying the risks and uncertainties concerning humans and the environment at an early phase of the innovation process. The SbD approach addresses the safety of the material/product and associated processes through the whole life cycle within three pillars of design: safe(r) material/product, safe(r) production and safe(r) use and end-of-life.

These principles underpin frameworks for alternative assessment for safer chemicals. Due to a growing concern regarding sustainability of chemicals, environmental aspects have been gaining more prominence and they are starting to be considered in addition to chemical safety in frameworks for assessment of alternatives.

2.3 Life Cycle Assessment

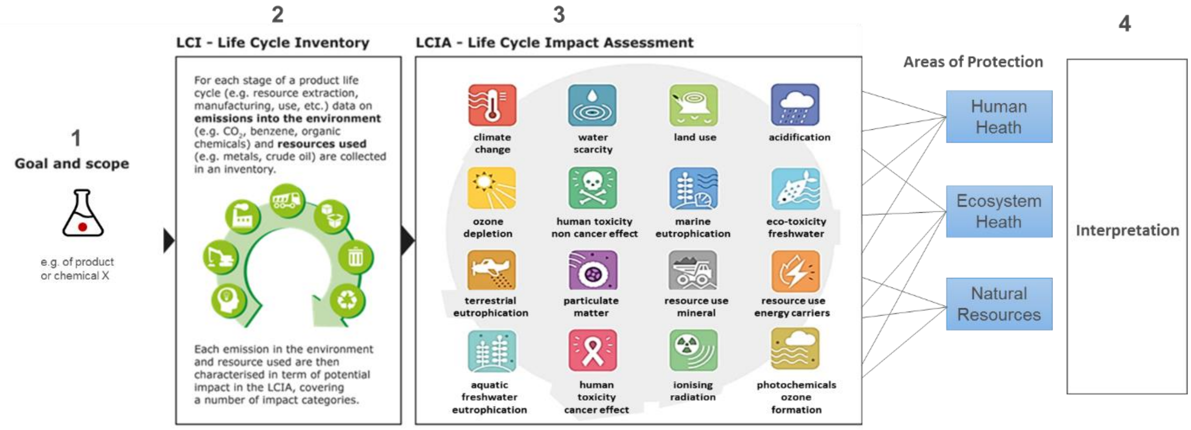
Assessing sustainability requires integrated approaches, able to model complex systems and to capitalise the best knowledge on impact assessment. Moreover, they should allow comparison between different options, be reproducible and transparent, highlighting trade-offs. Among the available approaches to sustainability assessment, Life Cycle Thinking (LCT) and the life cycle-based approaches applying LCT can play a pivotal role in comparing options and solutions in terms of sustainability (Sala et al., 2013a). Life cycle thinking is a basic concept referring to the need of assessing burden and benefits associated to products/sectors/projects adopting a holistic perspective, from raw material extraction to end of life. LCT can be applied to assess the environmental, social, and economic pillars using the Life Cycle Assessment (LCA), the Social Life Cycle Assessment (S-LCA), and the Life Cycle Costing (LCC) methodology. The Life Cycle Sustainability Assessment (LCSA) combines the three above mentioned methodologies to provide a holistic assessment of the implications of a product life cycle. The three methodologies have various levels of availability and maturity, which in turn influence their level of implementation (Valdivia et al., 2021). LCA is the most established and mature methodology, having implemented characterisation models with justified impact pathways. A compendium on LCA providing guidance on how to apply LCA is provided by Hauschild et al. (2018). S-LCA and LCC are less developed, especially concerning the impact assessment phase.

The importance of employing a life cycle perspective in assessing sustainability of production and consumption systems has been increasingly acknowledged in the EU policies since the early 1990ies (Sala et al., 2021). The European Green Deal (EC, 2019a), for instance, includes several policy initiatives which explicitly cite and mention LC thinking and methods. In the Chemical Strategy for Sustainability (EC, 2020a) a life cycle perspective is required in the identification and minimisation of potential negative impacts linked to chemicals and materials.

Figure 6 shows the main elements of the LCA methodology, an internationally standardised tool (ISO, 2006) for the integrated environmental assessment of products (goods and services). As for the other LC-based methodologies (i.e., the Social Life Cycle Assessment and the Life Cycle Costing) four main phases are included in the methodology:

1. **Goal and scope**: describing the reason for executing the study, a definition of the studied product and its life cycle and the defining of system boundaries;
2. **Inventory**: listing all emissions released into the environment and resources extracted from the environment along the whole life cycle of the product under investigation;
3. **Impact assessment**: results or indicators of potential environmental and human health impacts are translated, with the help of an impact assessment method, into environmental impacts;
4. **Interpretation**: necessary for identifying, quantifying, checking and evaluating information from the results of the inventory and/or the Life Cycle Impact Assessment.

Figure 6. Main elements of the Life Cycle Assessment methodology



For each stage of a product life cycle (e.g. resource extraction, manufacturing, use, etc.) data on **emissions into the environment** (e.g. CO_2, benzene, organic chemicals) and **resources used** (e.g. metals, crude oil) are collected in an inventory.

Each emission in the environment and resource used are then characterised in term of potential impact in the LCIA, covering a number of impact categories.

2.4 Sustainable Innovation and Responsible Research and Innovation

Aside principles that guide the development of SSbD chemicals and materials as for example the green chemistry principles or circular chemistry and tools that assess the performance of chemicals and materials allowing to identify those that are SSbD such as Life Cycle Assessment, other key concepts underpinning the SSbD framework are **Sustainable Innovation**, which are those innovations that can reconcile economic, social and environmental goals in order to achieve a “win-win-win” situation (Afeltra et al. 2021) and **Responsible Research and Innovation** (RRI).

Innovation can take many forms, for example product innovation (change in products/services offered by a company), process innovation (change in the way products/services are offered or presented to the consumer), the innovation of position (change in the context in which the products/services are introduced in the market) and paradigm innovation (change in the basic mental models that guide the actions of the company) (Iakovleva et al. 2021). There is a growing literature referring to RRI (Yaghmaei et al. 2021), which is framed as a way to steer and manage innovation development, and to connect the basic concerns of business with the global challenges of society, i.e., the challenge for companies in this increasingly competitive world to innovate in order to generate economic benefits, but also to generate sustainable social value. Definition of RRI includes ‘Responsible innovation refers to a new or significantly improved product, service, or business model whose implementation at the market solves or alleviates an environmental or a social problem’ (Halme et al. 2014). Hence, principles of RRI include anticipation of societal needs and reflection of concerns (Owen et al. 2012), which calls for new innovation policies. The RRI has led to the development of a possible framework of implementation, including for SMEs (Gonzales-Gemio et al. 2020).

3. Definitions and sustainability dimensions in the proposed SSbD framework

In this section, the definitions adopted in the framework and the sustainability dimensions addressed are presented. Annex 1 gives an overview of the definitions of the terms used.

3.1 Definitions

Sustainability and safety

When applied in the context of chemicals/materials, the concept of **sustainability** could be formulated as **the ability of a chemical/material[7] to deliver its function without exceeding environmental and ecological boundaries along its entire life cycle, while providing welfare, socio-economic benefits and reducing externalities.**

The **safety** concept is transversal to all sustainability dimensions (environmental, social and economic) and it is related to the absence of unacceptable risk (in line with REACH art 68 (EU, 2006)) for humans and the environment, **preferably ensured by avoiding chemicals with intrinsic hazard properties**.

Chemicals and materials

The focus of this report (aligned with the CSS) is on the development of a framework to define SSbD criteria for chemicals and materials. The term 'chemical' has different interpretations. REACH (EU, 2006) and CLP (EU, 2008), the basis for EU chemicals legislation, do not define 'chemical', but use, defines and distinguish the legal terms 'substance[8]' and 'mixture[9]' for chemicals. However, in daily practice, people often make an intuitive distinction between 'chemicals' and 'materials'. To facilitate general understanding, and ensure comprehensiveness, the SSbD criteria developed in this report refer to both chemicals and materials[10] .

It is important to assess the sustainability of the use of the chemical or material in the final application e.g. where it is used as a part of or as an ingredient in a product[11]. However, there are many sustainability aspects associated with a product that are not related to its ingredients or components and that need to be taken into account when evaluating the sustainability of a product. This report is limited to a framework for the definition of SSbD criteria for chemicals and materials; it does not apply for the definition of criteria for 'products'.

'By-design' (re-design)

In the context of SSbD criteria definition for chemicals and materials, the term 'by-design' can be interpreted at 3 levels:

- Molecular design: this is 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 be safe(r) and (more) sustainable.
- Process design: this is the design of new or improved processes to produce 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.

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[7] This definition ca also be applied to products and services

[8] 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'. Please note that a 'substance' can have a very complicated chemical composition, for example creosote, which is produced by the distillation of tar from wood or coal, is a substance. (EU, 2006)

[9] Mixture: 'a mixture or solution composed of two or more substances' (EU, 2006)

[10] Material = denote 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 (EC, 2021e)

[11] see definition in Annex 1

- Product design: this is 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.

The SSbD framework proposed in this report covers all three levels. It can be used to determine into which direction molecular design should go (including designing an optimal production process), but it is also intended to be useful for the engineers and scientists improving or inventing new production processes (re-design) for already existing chemicals and materials, and for product designers, when they need e.g. to select different chemicals and materials to meet the functional demands of the product under development.

Criteria

A criterion is defined as an aspect (e.g. climate change) with an assessment method and a minimum or maximum threshold or target values, on which a decision may be based.

The SSbD criteria for chemicals and materials will be used to assess the overall sustainability of the use of a particular chemical or material with a specific function in a particular application. Where SSbD is applied to more than 1 chemical or material, any comparison among chemicals/materials will be based on (strictly) equivalent functionality. Therefore, also the amount of chemical/material used to achieve a particular function, which may need a larger amount of chemical A than of chemical B, should be taken into account.

3.2 Sustainability dimensions

Ideally, an SSbD framework encompass all sustainability dimensions. The main sustainability guidance and global objectives (e.g. the sustainable development goals) (UN, 2015), as well as the review of the dimensions addressed by existing frameworks (Caldeira et al. 2022) identified the following sustainability dimensions:

- Safety
- Environmental
- Social
- Economic

As mentioned above, **safety** is an integral element of sustainability that refers to human health and environmental safety aspects of chemicals and materials. In the context of chemicals assessment, safety could be referring to a certain condition where a stressor (e.g. a chemical) is unlikely to cause any adverse effect to a receptor (e.g. humans and other organisms) (more related to intrinsic hazard properties of the stressor) or where a receptor is protected from risk (more related to control measures or mechanisms to minimise exposure to the stressor). In any case, the term safe involves receptors, and with that generally also requires the consideration of the contact (i.e. exposure) between stressors and receptors as addressed in a risk assessment context.

Current EU chemicals legislation is to a large extent based on the need to protect human health and the environment from the risks associated with the production and use of hazardous chemicals, i.e. on **'chemical safety'**. In the context of CSS and this report, 'safety' is to be interpreted as 'chemical safety', and refers to issues that may arise from their intrinsic hazard properties as well as during the production, the use phase or at the end-of-life of the chemical/material

Conceptually, (chemical) safety and sustainability are not unrelated: **chemical safety is an essential element of sustainability**. Chemical pollution[12] and toxicity of chemicals to human health and the environment are obvious threats to environmental and social sustainability, and the political, economic and legal risks associated with working with hazardous chemicals or critical raw materials are aspects of economic sustainability.

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[12] Defined as the presence or increase in our environment of chemical pollutants that are not naturally present there or are found in amounts higher than their natural background values (see Annex 1 for source)

Within the safety dimension, several aspects are covered, from the **intrinsic hazardous properties** of the chemical or material to **safety of the production and processing** and **safety of chemicals/materials final application**. In this report, safety is treated as the first aspect of sustainability, onto which other sustainability elements are subsequently added. This supports an efficient use of assessment resources by a step-wise increasing assessment scope, in line with several approaches proposed in literature (Fantke et al. 2020; IC2, 2017; Rossi et al. 2012; Wang and Hellweg, 2021).

Environmental sustainability refers to the ability to conserve natural resources and protect global ecosystems to support human health and wellbeing, within the limits of our Planet. Assessing environmental sustainability implies to assess the environmental impacts generated by chemicals/materials along the entire life cycle to move towards:

- A **toxic-free environment** as stated in the CSS (i.e. minimising the total toxicity footprint in terms of ecotoxicity and human toxicity[13] - at each stage of the production and consumption life cycle, originated not only by the assessed chemical or material, but also by all the chemicals that are emitted along the life cycle[14]) (EC, 2020a);
- A **climate-neutral economy** (i.e. minimising the emission of greenhouse gases along the life cycle) (EC, 2019b);
- A **resource efficient economy** and a **regenerative economy** (i.e. using natural resources in a sustainable manner, minimising inputs and waste generation, and providing more benefits than burdens) (EC, 2020b);
- The **reduction of biodiversity loss** and the conservation of ecosystem functioning, addressing the main drivers of structural and functional biodiversity loss (e.g. land use, climate change) (EC, 2020c);

An additional aspect is related to the ambitions that the "EU needs to accelerate the transition towards a regenerative growth model that gives back to the planet more than it takes" (EC, 2020b). The **regenerative economy** considers the potential that a chemical or material has to produce environmental benefits at system level (i.e. outside the boundary conditions of the whole life cycle of the chemical/material), when applied in a specific context. Under a regenerative economy concept, a **chemical or material** should provide benefits well beyond the burdens that is generating for its production and use. This could be related to a number of cases, such as:

- a chemical/material designed for reducing environmental pollutions (e.g. Dave and Chopda, 2014);
- a chemical/material that when applied is reducing the environmental burdens of the system where it is applied (e.g. a lightweight material which is reducing fuel consumption in a vehicle, so the overall carbon footprint of the system);
- a chemical/material which allows to reduce and substitute virgin resources to preserve and regenerate ecosystems[15].

These additional benefits could be assessed with life cycle assessment, and some illustrating case studies are reported, e.g. in ICCA (2017).

The SSbD framework announced in the CSS is focused on the environmental dimension of sustainability, i.e. acting in ways that do not exceed the Earth's ecological limits. However, sustainability covers as well social and economic aspects.

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[13] Note that, as stated above, this refers to eco-toxicity and human toxicity impacts due to emissions originated by e.g. raw materials extraction and processing of chemicals and materials (and the further processes) that impact humans and other organisms due to their distribution via environmental compartments (e.g. soil, water, air) and not (eco-) toxicity of the chemical/material as such.

[14] For example, the chemical emitted in the raw material extraction, or those due to the energy use during chemical manufacturing etc.

[15] As mentioned on page 1 of the Circular Economy Action Plan (CEAP) (EC, 2020b).

Social Sustainability is well reflected in the SDGs framework which comprises a globally agreed list of objectives and targets to be pursued for achieving sustainable development. In the SDGs framework several Goals focus on social aspects, e.g. poverty eradication (SDG 1), food security (SDG 2), health (SDG 3), education (SDG 4), gender equality (SDG 5), decent work (SDG 8), reduce inequalities (SDG 10), peace and justice (SDG 16). Other SDGs, while referring to environmental or technological aspects, have a clear link with social aspects, like those related to water and sanitation (Goal 6) and access to energy (Goal 7).

Economic sustainability refers to multiple aspects related to techno-economic feasibility, to operational costs, etc. Moreover, there are important considerations to be made in the context of SSbD such as the 'availability' of raw materials, as chemicals/materials cannot be declared SSbD if the raw materials to produce them are not renewable or are (very) scarce and extracted and processed in an unsustainable manner. Economic aspects play a role when there is a need to rank chemicals and materials based on SSbD criteria (even if they are not SSbD). However, mainly externalities consideration is at stake in a sustainability framework like the SSbD one.

3.3 Hierarchical approach to SSbD dimensions

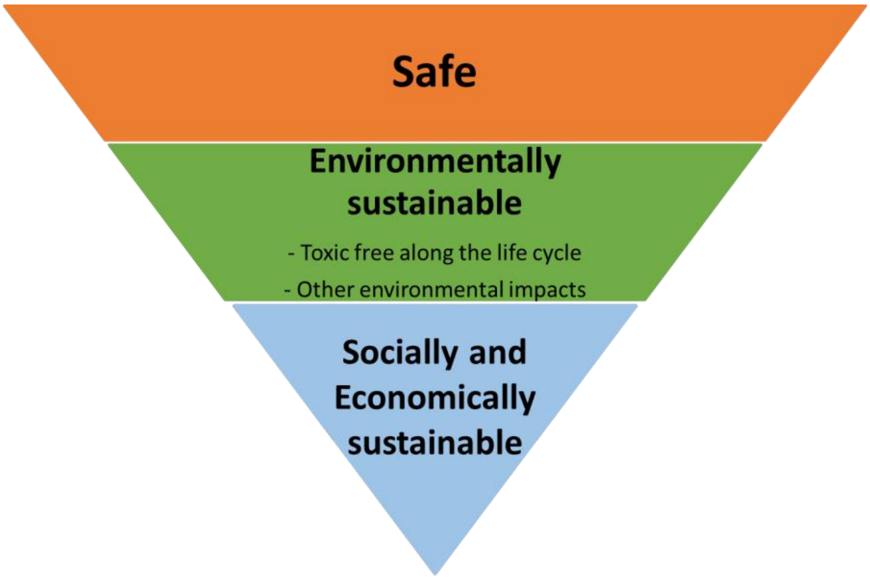
Considering the above, the proposed SSbD framework to assess chemicals and materials follows a hierarchical approach as illustrated in Figure 7 in which safety aspects are considered first, followed by environmental, social and economic aspects. This is in line with several approaches proposed in literature (Fantke et al., 2020; IC2, 2017; Rossi et al., 2012; Wang and Hellweg, 2021) as well as with policy priorities (EC, 2021d). The first step is to ensure safety by considering chemicals/materials with certain hazards properties as non-sustainable even if they are following green principles and have a relatively low environmental impact (e.g. the chemical production is at low energy-intensity) (Fantke et al., 2020). This rationale, which is aligned with the CSS, allows setting priorities and avoiding trade-offs on specific safety aspects (that are defined as cut-off criteria as explained in section 4.2.1), thus making the process more consistent and efficient. In this way, specific safety aspects frame the chemical/material development within which sustainability could be optimised, following the considerations regarding the functionality.

In this context, the framework proposes to assess safety in the first place considering the previously mentioned elements, i.e. chemical/material hazards, production safety, and direct exposure impacts. If the minimum criteria for this safety dimension are met, then the assessment can proceed to evaluate the environmental sustainability dimension by environmental life cycle assessment including toxicity (indirect impacts, see footnote 9) and other environmental impact categories and after that, the social and economic dimensions. Techno-economic considerations are normally considered by companies when developing a new chemical/material to decide whether to go further or not with its development. So, the proposed framework goes beyond this layer of analysis internal to the company, focusing more on externalities.

This rationale is reflected in a stepwise approach presented in section 4.2, which intends to reduce the burden of assessment as the initial steps propose to identify 'prohibitive' issues. For example, if the chemicals exhibit safety issues regarding direct exposure impacts, an LCA would only be performed after addressing the problem encountered. Nevertheless, depending on the practice of each organisation, the different steps could be assessed simultaneously. In the proposed framework, when the chemical/material passes the criteria for safety and environmental sustainability it is considered SSbD. If the minimum criteria for the safety dimension are not met, then the chemical/material cannot be considered as SSbD.

Details on the structure of the framework and on how to define criteria for safety and environmental sustainability to identify SSbD chemicals/materials are provided in the following section.

Figure 7. Hierarchical principles underpinning the SSbD framework suggested



4. Structure of the framework: a stepwise approach

The EU CSS calls for the development of SSbD criteria for chemicals/materials to be defined through a holistic framework integrating the minimisation of the environmental footprint of chemicals/materials with their safety and function throughout their entire lifecycle. In particular, the framework shall support the development of new chemicals/materials and substitution of existing ones that are toxic to humans or the environment, persistent, bio-accumulative or mobile (the latter is undesirable in combination with toxicity or bioaccumulation). These priorities, which should be reflected in the proposed SSbD criteria, are defined at EU level and address many different properties also beyond substances of very high concern (SVHC).

The SSbD framework proposed is a **general approach for the definition of criteria for SSbD for chemicals and materials**. It is broadly applicable allowing the definition of a set of operational criteria that can be implemented and that increase or ensure compliance with reference targets for safety and sustainability of chemicals and materials. It can be **applied to newly developed chemicals and materials or to existing ones**. For the latter, the framework can be used i) to support the redesign of their production processes by evaluating alternative processes to improve their safety and sustainability performance, or ii) to compare them on the basis of SSbD criteria (e.g. for innovation by substitution with better performing chemicals/materials, in terms of safety and sustainability, or selection in downstream application).

Aligned with the CSS, the framework foresees the assessment of the **entire life cycle of a chemical or material**, including the design phase and considering among others its functionality. Functionality is a key element to be considered in the alternative assessment of chemicals and materials as highlighted in some of the most recent frameworks for chemical alternative assessment (Cefic, 2022). This approach is sometimes called **functional substitution** referring to the idea of comparing chemicals not only on the base of chemical structure or physico-chemical properties, but also in the context of their final use to avoid regrettable substitution (Tickner et al. 2015).

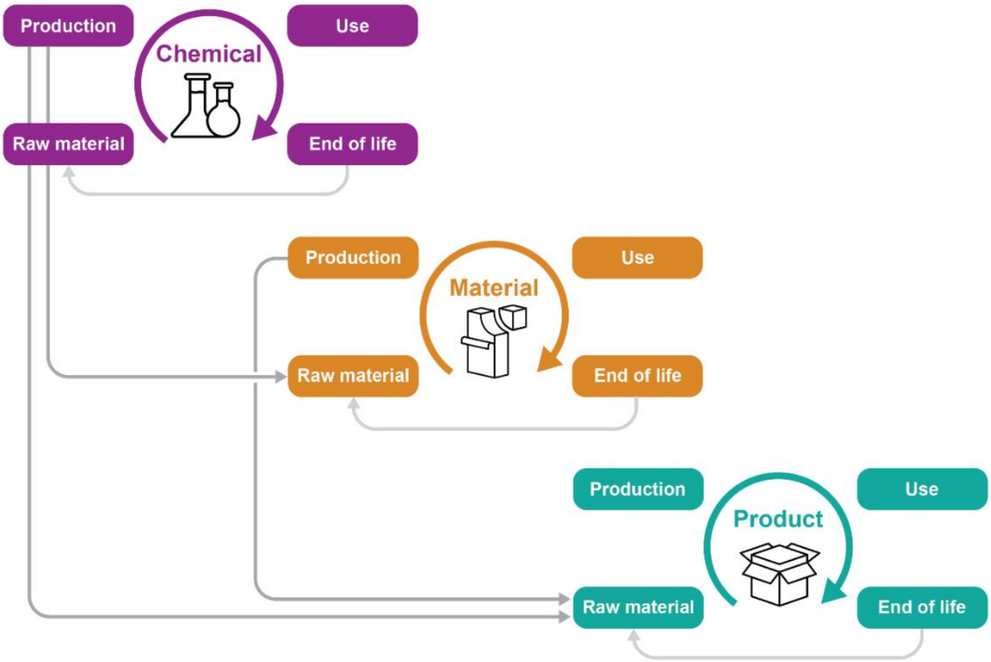
This concept is also reflected in **LCA** with the definition of **functional unit**, which is the quantified performance of a chemical/material required to provide a specific function and is the basic requirement for meaningful comparisons in LCA. The functional unit of an LCA can be defined answering 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? Following this concept, the reference flow is the amount of a chemical/product that is needed to fulfil the functional unit. Therefore, in LCA the comparison of two chemicals/materials is always done regarding their function, using the appropriate reference flow for each chemical/material. For this reason, even if the evaluation of *products* is outside the scope of this framework, the use of the *chemical/material* under assessment in products is considered to define the functional unit as illustrated in Figure 8.

For example, for a plastic additive such as a plasticiser (chemical/material under assessment), the functional unit could be defined as the ability of a plasticiser, when added to Polyvinyl Chloride (PVC) to produce a polymeric food contact film (product) with a defined level of flexibility (i.e. the extent of the function provided, measurable with one or more defined physical or chemical properties) for a required service life ("How long?") without leaking out of the PVC ("How well?"), while the reference flow will be the amount of a specific plasticiser required to achieve this functional unit.

When searching for alternatives using a functional substitution approach, it is important to **investigate solutions also beyond 'chemical for chemical' substitution**. In the example of the flexible PVC film above, the aim of substitution is avoiding a hazardous plastic softener (i.e. phthalate). The alternatives could be e.g. an alternative non-hazardous softener, to replace PVC with another type of plastic that is inherently flexible, to generate packaging from another type of material or to conclude that packaging may not be needed.

It is important to note that the design of an alternative delivering a certain function can be also addressed by exploring non-chemical /material alternatives. This report refers exclusively to the case in which a chemical or material alternative is assessed.

Figure 8. Simplified representation of the life cycle of a chemical and its use in the life cycle of materials and products. The life cycle stages are connected via logistics (transport and distribution stages)



To support the development of a SSbD chemical/material, certain principles should be followed in the design phase. Therefore, as illustrated in Figure 9 and described below, the SSbD framework entails two **components**:

1. a **(re)design phase** in which design guiding principles and indicators are proposed to support the design of chemicals and materials, and
2. a **safety and sustainability assessment** phase in which the safety, environmental and socio-economic sustainability of the chemical/ material are assessed. Socio-economic aspects are included in the framework to be explored as methods still need to be further developed.

It is important to highlight that **design principles are provided as guidance** (section 4.1) nonetheless the **objective of the framework is to ensure that SSbD criteria are developed/fulfilled in accordance with the sustainability assessment**. The later, presented in section 4.2, consists of five steps.

The **sustainability assessment** allows the identification of SSbD chemicals and materials, in particular how criteria can be defined. It comprises 5 Steps that can be carried out sequentially or in parallel, depending on the data and tools availability and the specific purpose of the exercise. Moreover, the assessment can be done and, in many cases, should be done iteratively to optimise the results.

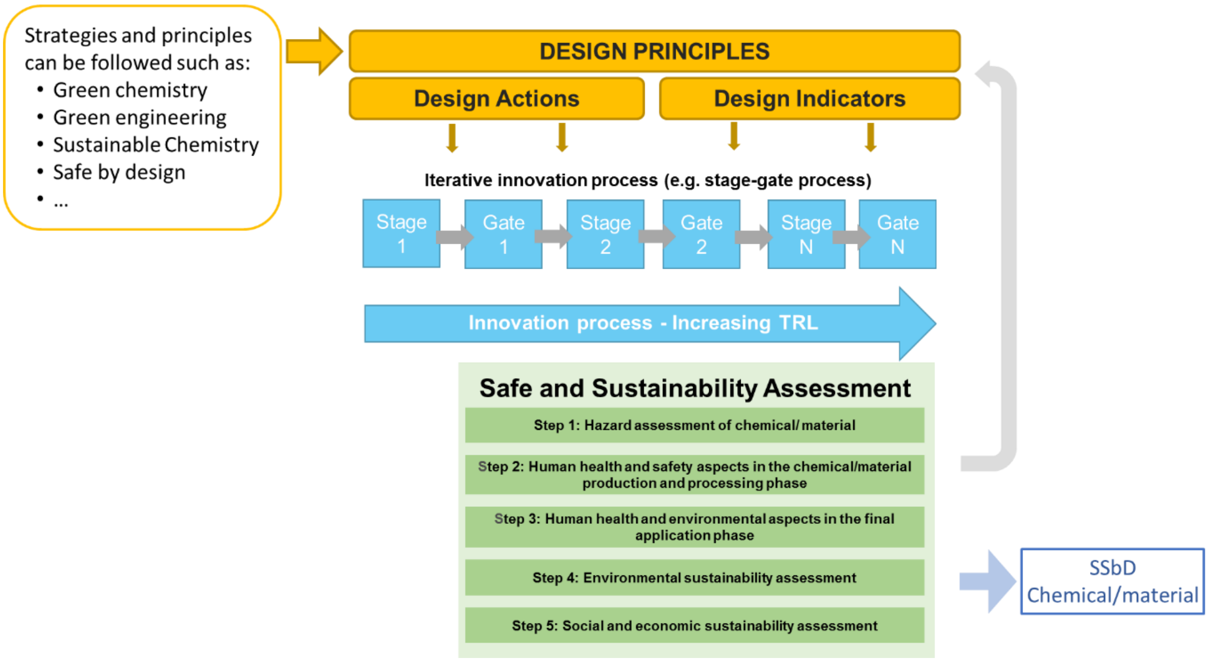
The safety and sustainability assessment will allow the evaluation of a chemical/material in terms of fulfilling SSbD criteria, in line also with the design principles (see below). In case the assessment indicates a poor performance of the chemical/material against the criteria, a redesign of the chemical, its production process or its application (use) is needed to improve the sustainability (Figure 9, grey arrow).

4.1 Guiding Design principles for SSbD: integration of SSbD assessment in the innovation process

The concept of 'safe and sustainable by design' implies the design (or redesign) of safe chemicals and materials, minimising their emission into the environment and the use of natural resources with the aim to reduce the negative impacts to human health and environment. During the design phase of a chemical/material, a number of principles can support the integration of SSbD considerations. This can be done in an iterative process of continuous improvement associated to the innovation process adopted in each organisation. These principles can be applied through specific actions and monitored with quantitative indicators with the goal of improving different aspects of safety and sustainability simultaneously.

The development of a new chemical/material is often brought on through an innovation process that can be structured in stage-gate[16] approach. The process development can be monitored using the Technology Readiness Level (TRL) and at each stage quantitative and qualitative new information may be available for the assessment. This process can interact with the present framework using the design principles, actions and indicators described in this section as illustrated in Figure 9. The safety and sustainability assessment (green box, figure 9) should be performed at early TRL (to the extent possible) to ensure that the application of the principles is indeed resulting in a good performance. It has to be noted that the focus of this report is on the development of criteria for SSbD chemicals/materials and not on the innovation process itself. Therefore, the principles, actions, and indicators presented here can be adapted by the developers to suit their innovation purposes. An example of the integration between innovation workflow and SSbD can be found in CEFIC's guidance (Cefic, 2022) or in the NanoReg2 project (Jiménez et al. 2022).

Figure 9. Integration of SSbD in the innovation cycle including principles to be considered in the design phase of SSbD chemicals and materials, whose safety and sustainability performance is verified with the assessment allowing the classification of the chemical/material as SSbD. TRL: Technology Readiness Level



The proposed design principles (Table 1) build upon those developed in different contexts, e.g. in green chemistry (GC) (Anastas and Warner, 1998), green engineering (GE) (Anastas and Zimmerman, 2003), circular chemistry (CC) (Keijer et al. 2019), the Golden Rules (GR) developed in UBA (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, 2018a), to zero pollution (EC, 2021d) etc.). Many of these principles include both safety and resource related aspects and intend to help the design or redesign of chemicals, materials, and related processes. The complete list of the principles used to compile this SSbD set, as well as the definitions and the sources are reported in Annex 2. The list is illustrative and not exhaustive. It could be expanded in relation to the specific sector or type of chemical and materials. For example, Cefic suggests other design

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[16] Stage-gate approach is a general system for innovation process. A stage is the part of the project in which the work is done to prepare a set information and deliverables. The gate is the activity in which the management validates the quality of the collected information or make decisions according to the deliverables and results of the stage. The gate can be used as a quality check for data collected in the stage activities before moving to more expensive stages or as a filter to bring on only the most promising projects (Cooper, 2010).

principles related to safety and sustainability along with additional considerations (Cefic, 2022); the EU project Orienting (Bachmann et al, 2021) is a critical review of different circularity indicators available in literature and it illustrates product circularity strategies; the European Taxonomy (Platform on Sustainable Finance, 2022a,b) lists activities and proposes technical criteria for the chemical industrial sector.

Among the principles, some are related to environmental sustainability and resources (e.g. SSbD 4, 7 & 8), aiming to minimise the use of natural resources and the emission of substances into the environment. This can be achieved by several strategies which include, for example, increasing the resource efficiency, the process efficiency (e.g. via process intensification or applying lean thinking), applying the waste hierarchy (reduce-reuse-recycle), using innovative business models for innovation, exploring opportunities for industrial symbiosis etc. (Corona et al. 2019).

Moreover, Table 1 presents actions regarding the principles that can be adopted in the design (re-design) phase as well as indicators that can be used to measure the adoption of such principles and provide insights into e.g. the circularity of the system. For example, to measure the level of application of these strategies, in SSbD principles 4, 7 & 8, specific indicators related to circularity are suggested (i.e., Value-based resource efficiency indicator (VRE), Material Circularity Indicator (MCI), Recycled Content).

As mentioned, the adherence to such principles does not allow to conclude on the sustainability performance of the chemicals and materials. For that, a safety and sustainability assessment should be conducted. The safety, environmental and socio-economic sustainability performance of the chemicals and materials designed following these principles should be assessed, including to which extent they comply with specific safety and sustainability criteria (ECHA, 2021a; Sheldon, 2018).

This is particular important when dealing with the circularity of the system. While the circularity aspect is captured by some of the principles and indicators, the actual improvement in the environmental performance is measured through the sustainability assessment. For example, if a 'primary non-renewable feedstock used for the production of a chemical/material is replaced by a secondary one (i.e. recycled or waste-based), this leads to the reduction of the extraction and use of a non-renewable resource (e.g. fossil feedstock for production of virgin plastic) and improvement of the circularity of the system. However, it should be noted that using secondary feedstock does not automatically imply that the overall environmental impact of the system is lower, since the process for waste collection, production and transport of the recycled feedstock may produce more environmental impacts or safety concerns than the use of the primary one, or since recycled materials may contain residues of (harmful) chemicals on top of newly added chemicals in each recycling step (Fantke and Illner 2019).

Similarly, for the use of renewable resources, such as biomass feedstock, the environmental impacts are often strongly affected by the biomass sourcing. The environmental sustainability profile of chemicals and materials derived from secondary biomass (for example a by-product or residues of other industries (e.g. agri-waste, food-waste or forestry residues) or other types of biomass waste), can differ from when primary biomass (grown on arable land) is used. The latter will have an effect on environmental sustainability aspects such as land use and land use change (direct and indirect), biodiversity loss, or social issues as competition with food production. Another example is related to the use of non-renewable abiotic resources, such as the ones included in the list of Critical Raw Materials (CRM). For these materials, the comparison at mass level as suggested in one of the indicators proposed in Annex 2 can be helpful to keep track of reduction in use of CRM among different process designs, but it is not exhaustive, since it does not consider the specific availability of each resource. The accounting of CRM mass gives therefore an economic (rather than environmental) information and could eventually support decision making for the substitution of critical materials. The use of the impact category called “Resource use, minerals and metals” gives to each of them a characterisation factor based on the scarcity, therefore allowing a comparison.

Therefore, the safety and sustainability assessment is needed to take into account all these different aspects to give a more comprehensive picture.

Table 1. 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 (see Annex 2 for 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.	- 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 the production process - Minimize waste generation - Identify occurrence of use of Critical Raw Material[17], towards minimizing or substituting them	- Net mass of materials consumed (kg/kg) - Reaction Yield - Atom Economy - Material Intensity index - 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 completely avoid using hazardous chemicals/materials where possible.	- Reduce and/or eliminate hazardous chemicals/materials in manufacturing processes - Verify possibility of using hazardous chemicals/materials in close 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)
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 (%)

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[17] 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 (see Annex 2 for definition)**
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 hazardous emissions or pollutants in 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)	Eliminate exposure to chemical hazards from processes as much as possible. Substances which require a high degree of risk management should not be used 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 value chain-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. Design for preventing the hindrance of reuse, waste collection, sorting and recycling/upcycling.	- 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): - 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	- Recyclable? (yes/no) - Durability (years) - Disassembly/reparability design (yes/no)

SSbD principle (based on)	Definition	Examples of Actions	Examples of indicators related to the SSbD principle (see Annex 2 for definition)
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 -Applying responsible sourcing principles	- 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)

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). See Annex 2 for information on the principles

4.2 Safety and Sustainability assessment

This section presents the safety and sustainability assessment to be performed for the identification of SSbD chemicals and materials, in particular how criteria can be defined.

The safety and sustainability assessment is composed of five steps from which the first three steps cover different aspects and angles of chemicals/materials safety, step four deals with the environmental sustainability aspects, while step five cover the social and economic dimensions. The steps, even though presented sequentially, can be performed in parallel, as information becomes available along the life cycle of the chemical/material and depending on the specificity of the assessment (e.g. on a new or an existing chemical/material). Moreover, the assessment can be done and, in many cases, should be done iteratively to optimise the results. The steps are:

- *Step 1 – Hazard assessment of the chemical/material (intrinsic properties)*

  The first step looks at the intrinsic properties (Figure 10 (a)) of the chemical or material in order to understand its hazard [18] profile before further assessing the safety during use.

  One of the reasons for implementing hazard-based criteria as a first step in the SSbD framework, is that 'safe and sustainable by design' chemicals should be inherently safe to use in all kinds of uses (including unforeseen uses) in future life cycles. In this context the term 'by design' is interpreted and refers to intrinsic properties.

  In the design phase, not all possible uses of a chemical/material are known and they cannot be always predicted, therefore establishing a set of hazard-based criteria is needed that can guide the developers towards designing less hazardous chemicals or materials. There are many instances of hazardous chemicals present in recycled materials in which they were never meant to be present, see for example the case of hazardous flame retardants (ChemSec, 2021; Brosché et al., 2021; Straková et al., 2018) in toys and food contact materials. This is an example of a situation whose frequency would be significantly reduced by applying an SSbD approach. Based on these considerations, the exposure aspects are not part of this first step but are considered in the other assessment steps.

- *Step 2 – Human health and safety aspects in the chemical/material production and processing phase*

  In this step, the human health and safety aspects related to the chemical/material production and processing are assessed. It refers to production process from the raw material extraction (from natural resources) to production (e.g. substance manufacturing, mixing) of the chemical/material including the recycling or waste management (Figure 10 (b)).

  The goal is to assess whether the production and processing of the chemical/material poses any risk to workers. The assessment covers all the hazards of the chemicals/materials used in the process (raw chemicals/materials, processing aids…) and the potential for exposure of workers to them.

- *Step 3 - Human health and environmental aspects in the final application phase*

  In this step, the hazards and risks related to the chemical/material final application are assessed. It refers to use-specific exposure to the chemical/material and the associated risks.

  The goal is to assess whether the use of chemical/material in the final application poses any risk to the human health and the environment. The assessment covers the hazards of the chemical/material (Step 1) and the potential for exposure to humans and environment during the specific use (Figure 10 (c)).

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[18] Hazard is defined as a property or set of properties that make a substance dangerous (ECHA-term https://echa-term.echa.europa.eu/) or which has the potential to cause adverse effects to living organisms or to the environment (EFSA Glossary https://www.efsa.europa.eu/en/glossary-taxonomy-terms).

- *Step 4 - Environmental sustainability assessment*

  The fourth step considers environmental impacts along the entire chemical/material life cycle by means of LCA, assessing several impact categories such as climate change and resource use. Toxicity and eco-toxicity impact categories are also considered in this step, referring to impacts due to life cycle emissions from e.g. raw material extraction and processing of chemicals and materials (and the further processes) that impact humans and the environment via environmental compartments (e.g. soil, water, air), including mobility between compartments, and not via direct exposure (which is covered in step 3) (Figure 10 (d))

  The LCA covers all the life cycle stages, as the determination of whether a chemical/material is SSbD or not, includes considerations of its functionality, i.e. intended use. Therefore, for chemicals/materials as produced and placed on the market for further downstream diverse uses, it will be complicated, or even impossible, to determine if they are SSbD. Nevertheless, for these chemicals/materials an assessment can be done considering the stages up to and including production (i.e. 'cradle to grave'), and then allowing downstream users to apply this information to assess SSbD for their chemicals/materials. Nevertheless, following the proposed framework, these chemicals/materials can be assessed and compared in terms of performance but would not be classified as SSbD as this is only possible when considering the chemical/material specific application. This information will however be useful for downstream users of the intermediate chemical/material and can be included in a traceability scheme such as the Digital Product Passport (as a mechanism to transfer the information through value chains/communication channels) or in REACH. Moreover, main uses for the chemical/material can be identified and a preliminary screening of the SSbD results including application scenarios can be performed.

- *Step 5 - Social and economic sustainability assessment*

  The fifth step explores available approaches for the Social and Economic Sustainability assessment. In the case of social assessment, it describes which are the relevant stakeholders and social aspects that could be used for the social assessment. The economic assessment part focuses on non-financial aspects, e.g. the identification and monetization of externalities arising during the life cycle of a chemical or a material. These aspects are included in the framework to be explored as methods still need to be further developed.

Figure 11 illustrates the stepwise approach for the SSbD framework safety and sustainability assessment and Table 2 summarises the dimensions, aspects and respective system scope covered in the different steps.

The focus of this report is on how criteria for SSbD chemicals and materials can be defined. In the context of this work a criteria is an aspect with an assessment method and a minimum threshold or target values (on which a decision may be based). It is important to clarify that an aspect is measured via an indicator and several indicators can exist to assess the same aspect. Each indicator is measured with an assessment method. The following sections describing the steps are presented with the following structure:

i. a detailed description of which **aspects and indicators that can be used to measure such aspects and respective method,**

ii. a proposal for the **definition of criteria for each of the aspect** and

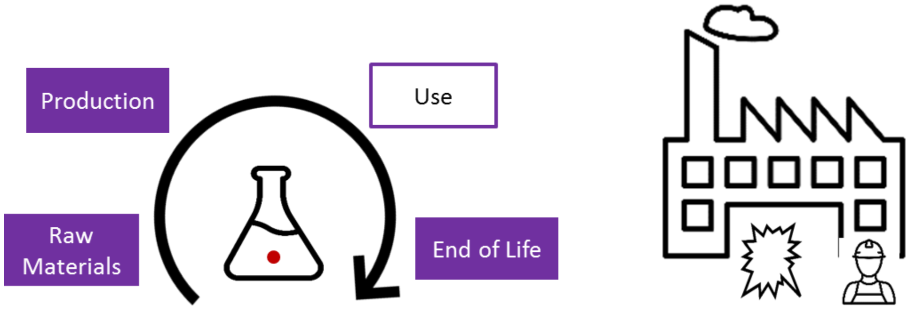
iii. an evaluation procedure (e.g. scoring system, levels).

As mentioned above, the steps can be performed sequentially or in parallel, depending on the specificity of the assessment and data availability along the life cycle of the chemical/material evaluated.

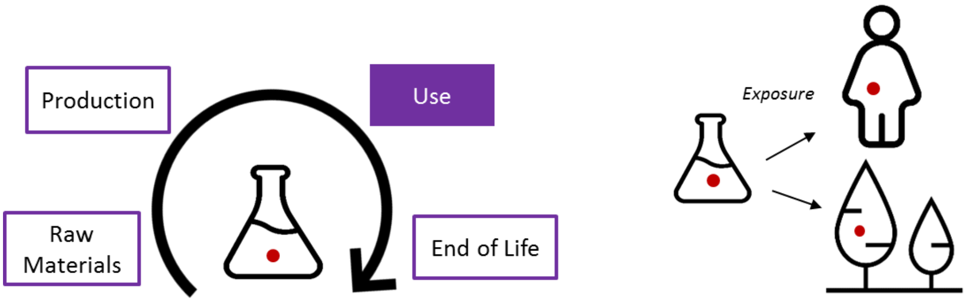
Figure 10. Illustration of chemical/material safety components captured in the proposed framework. Coloured boxes mean that life cycle stage is covered. The red dot refers to the chemical/material under evaluation while the orange/grey dots refer to all the other substances emitted along its life cycle (e.g. other toxic chemicals emitted in extraction of raw material or due to the energy use in manufacturing)

(a) Hazard properties of the chemical/material

(b) Hazards and risks related to the chemical/material production and processing



(c) Hazards and risks related to the chemical/material final application



(d) Environmental impacts along the entire chemical/material life cycle

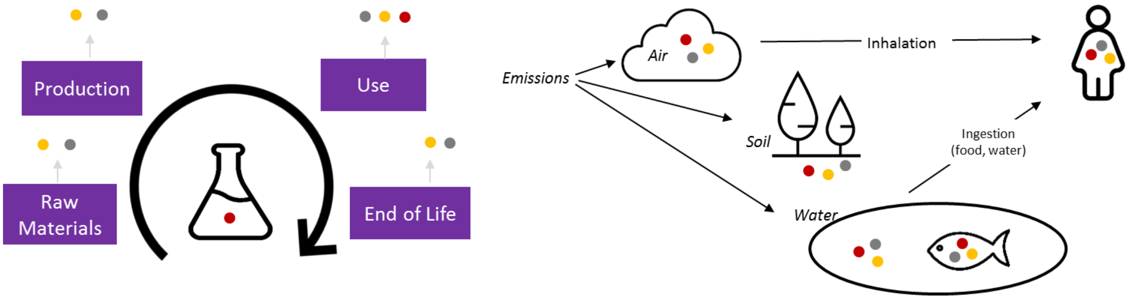


Figure 11. Stepwise approach for the SSbD framework safety and sustainability assessment. Note that step 5 is included in the framework to be explored as methods still need to be further developed

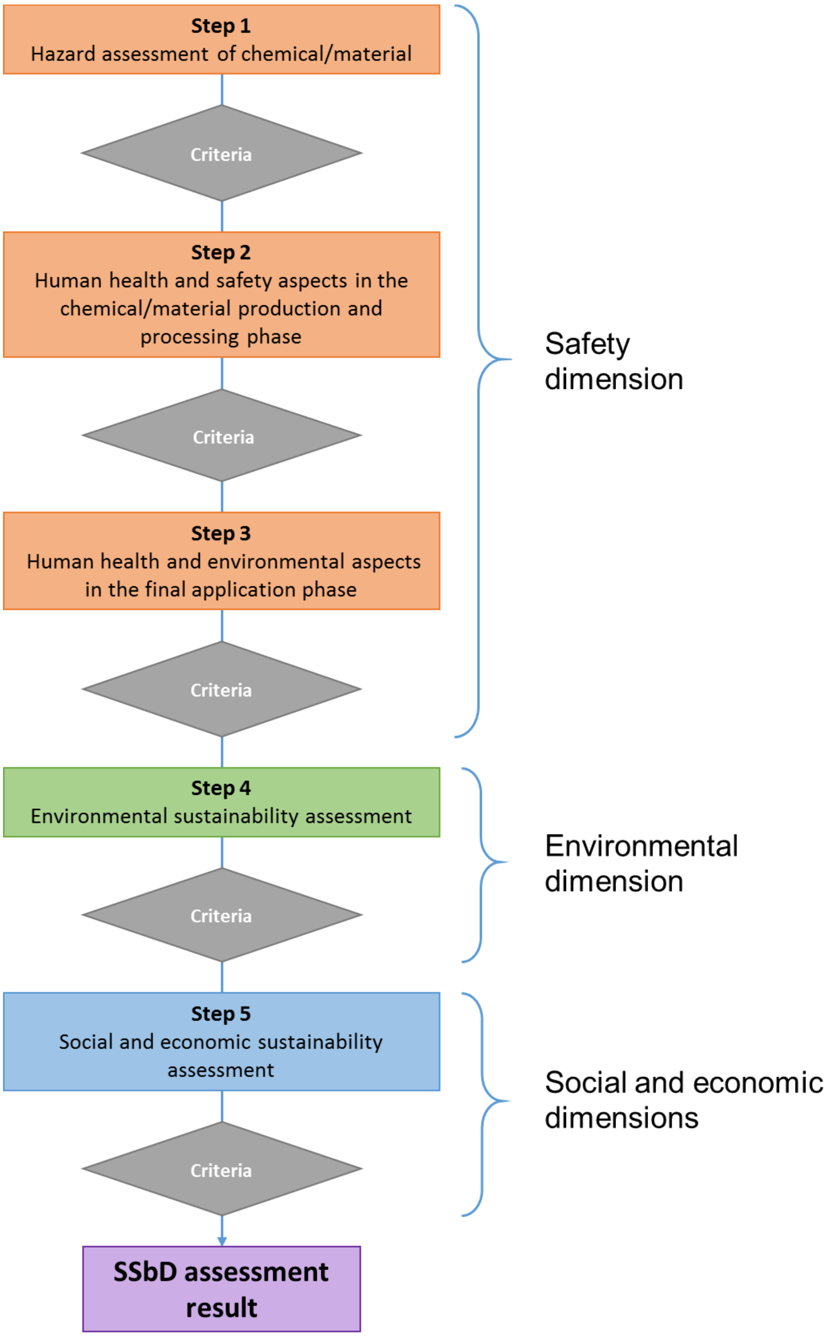


Table 2. Components of the proposed SSbD criteria definition framework

Step	Assessment Dimension	Assessment aspects	System Scope	Aspect/Indicator	Criteria
1	**Hazard assessment**	The assessment focuses on the hazard properties (human health, environmental and physical hazards) of the manufactured chemicals and materials	Chemical/Material intrinsic properties	See Table 3	See Section 4.4.1 and Table 4
2	**Human health and safety aspects in the production and processing phase**	Assessment of the human health and safety aspects during the production phase of the chemical/material from the used raw materials (production) and the manufactured chemical/material (processing, waste stage).	Chemical/material production and processing	See Section 4.2.2	See Section 4.2.2
3	**Human health and environmental aspects in the final application phase**	This step evaluates the human health and environmental impacts during the chemical/material final application phase.	Chemical/material application	See section 4.2.3	The indicator values should be below the safe levels. For details see section 4.2.3.
4	**Environmental sustainability (Life Cycle Assessment)**	Assess life cycle environmental impact categories for: Toxicity and Eco-toxicity Climate Change Ozone Depletion, Particulate Matter, Ionising radiation, Photochemical Ozone Formation, Acidification, Eutrophication Resources, Land Use, Water Use	Chemical/Material entire life cycle	See Table 7	Reduction by X% compared to the current state of the art for intended use. The 'X' might differ depending on the impact category. For details see section 4.2.4.
5	**Social Sustainability, Economic Sustainability**	This step is at an exploratory phase. It present an overview of social aspects that could be considered in the future. For the economic pillar, the step focuses on non-financial aspects, i.e. the identification and monetization of externalities arising during the life cycle of a chemical or a material.	Chemical/Material entire life cycle (for the economic part) Chemical/Material production and relevant suppliers (for the social part)	See Table 10 for examples	To de defined.

4.2.1 Hazard assessment of the chemical/material (Step 1)

In the context of the SSbD approach, the focus is first on the intrinsic properties of chemicals and materials and identifying those that are inherently hazardous. In the EU chemicals legislation, three main hazard classes are described, i.e. human health hazards, environmental hazards and physical hazards, and these classes are also included in the SSbD framework.

The goal here is to identify the most appropriate criteria that can be applied during the design (or re-design) of chemicals and materials in order to align with the overall objectives of the CSS, e.g.:

- Ensure that all chemicals and materials placed on the market are in themselves safe and that they are produced and used safely and sustainably (*point covered also by other components of the framework*)
- Ensure that final products do not contain the most harmful substances (e.g. that may cause cancer, gene mutation, affect the reproductive or the endocrine system, are persistent or bio-accumulative, those potentially affecting the immune, neurological or respiratory systems and chemicals potentially toxic to a specific organ)
- Drive the substitution of the substances of concern

The methodology includes the following:

- Definition of the aspects and indicators to be included
- Definition of criteria
- Evaluation system

Aspects and indicators

The aim is to establish a set of criteria and their indicators regarding the intrinsic properties[19] of chemicals or materials that can cause adverse effects to humans or the environment. The methodology for criteria definition is based on the hazard classes and categories established within the CLP regulation (Regulation (EC) No 1272/2008 (EU, 2008)) as well as REACH (Regulation (EC) No 1907/2006 (EU, 2006)). Three main categories of aspects are defined (Table 3) as follows:

- Intrinsic hazard properties relevant to human health (human health hazards)
- Intrinsic hazard properties relevant to the environment (environmental hazards)
- Physical properties (physical hazards)

Table 3 below aims to capture the aspects that need to be evaluated, as information becomes available along the life cycle of a chemical/material and in order to fulfil the criteria of Step 1. The grouping of the hazard properties is aligned with and follows relevant EC initiatives, such as the CSS (EC, 2020a), the proposal for a regulation regarding sustainable products (EC, 2022a) or the EU Sustainable Finance (Platform on Sustainable Finance, 2022c).

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[19] ECHA terms (https://echa-term.echa.europa.eu/): A characteristic of the chemical substance which can be used to determine its fate or to identify potential hazards. In order to register a substance under REACH, the registrant must submit specific information about the intrinsic properties of the substance in each of the following areas:

- physical/chemical properties
- human toxicological information
- ecotoxicological information

Data on the intrinsic properties of a substance are categorised into endpoints. For instance, 'carcinogenicity' is a human toxicological endpoint.

Table 3. List of aspects (hazard properties) relevant for Step 1

Group definition	Human health hazards	Environmental hazards	Physical hazards
Includes the most harmful substances (according to CSS (EC, 2020a)), including the substances of very high concern (SVHC) according to REACH Art. 57(a-f)[20],[21] (EU, 2006). These hazard properties form Criterion H1.	• Carcinogenicity Cat. 1A and 1B • Germ cell mutagenicity Cat. 1A and 1B • Reproductive / developmental toxicity Cat. 1A and 1B • Endocrine disruption Cat. 1 (human health) • Respiratory sensitisation Cat 1 • Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 1, including immunotoxicity and neurotoxicity	• Persistent, bioaccumulative and toxic / very persistent and very bioaccumulative (PBT/vPvB) • Persistent, mobile and toxic / very persistent and mobile (PMT/vPvM) • Endocrine disruption Cat. 1 (environment)	
Includes substances of concern, as described in CSS (EC, 2020a), defined in the Article 2(28) of SPI proposal (EC, 2022b)[22] and that are not already included in Criterion H1. These hazard properties form Criterion H2.	• Skin sensitisation Cat 1 • Carcinogenicity Cat. 2 • Germ cell mutagenicity Cat. 2 • Reproductive / developmental toxicity Cat. 2 • Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 2 • Specific target organ toxicity - single exposure (STOT-SE) Cat. 1 and 2 • Endocrine disruption Cat. 2 (human health)	• Hazardous for the ozone layer • Chronic environmental toxicity (chronic aquatic toxicity) • Endocrine disruption Cat. 2 (environment)	

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[20] Article 57(a) - carcinogenic category 1A or 1B; Article 57(b) - mutagenic category 1A or 1B; Article 57(c) - toxic for reproduction category 1A or 1B; Article 57(d) - persistent, bioaccumulative and toxic (PBT); Article 57(e) - very persistent and very bioaccumulative (vPvB); Article 57(f) - equivalent level of concern having probable serious effects to human health (and/or) the environment.

[21] Some substances with other hazard properties (e.g. STOT RE) may be classified as Substances of Very High Concern because of their 'equivalent level of concern' (see Article 57 (f) of the REACH Regulation)

[22] 'substance of concern' means a substance that:

(a) meets the criteria laid down in Article 57 and is identified in accordance with Article 59(1) of Regulation (EC) No 1907/2006; or

(b) is classified in Part 3 of Annex VI to Regulation (EC) No 1272/2008 in one of the following hazard classes or hazard categories:

- carcinogenicity categories 1 and 2,
- germ cell mutagenicity categories 1 and 2,
- reproductive toxicity categories 1 and 2, [to be added in the course of the legislative procedure once Regulation (EC) No 1272/2008 contains these hazard classes: Persistent, Bioaccumulative, Toxic (PBTs), very Persistent very Bioaccumulative (vPvBs); Persistent, Mobile and Toxic (PMT), very Persistent very Mobile (vPvM); Endocrine disruption],
- respiratory sensitisation category 1,
- skin sensitisation category 1,
- chronic hazard to the aquatic environment categories 1 to 4,
- hazardous to the ozone layer,
- specific target organ toxicity – repeated exposure categories 1 and 2,
- specific target organ toxicity – single exposure categories 1 and 2; or

(c) negatively affects the re-use and recycling of materials in the product in which it is present.

Includes the other hazard classes not part already in Criteria H1 and H2. These hazard properties form Criterion H3.	• Acute toxicity • Skin corrosion • Skin irritation • Serious eye damage/eye irritation • Aspiration hazard (Cat. 1) • Specific target organ toxicity - single exposure (STOT-SE) Cat. 3	• Acute environmental toxicity (acute aquatic toxicity)	• Explosives • Flammable gases, liquids and solids • Aerosols • Oxidising gases, liquids, solids • Gases under pressure • Self-reactive • Pyrophoric liquids, solid • Self-heating • In contact with water emits flammable gas • Organic peroxides • Corrosivity • Desensitised explosives

As mentioned above, the classification criteria for substances and mixtures established by CLP regulation (Regulation (EC) No 1272/2008) is used as reference and needs to be consulted for any detailed information. As an example, for the different hazard categories for carcinogens[23] mentioned in Table 3, the following definitions are used:

- Category 1A (Carc. 1A) - known to have carcinogenic potential for humans, classification is largely based on human evidence
- Category 1B (Carc. 1B) - presumed to have carcinogenic potential for humans, classification is largely based on animal evidence
- Category 2 (Carc. 2) - suspected human carcinogens

Regarding the **information requirements** to fulfil Table 3, a tiered approach should be applied, depending also on whether the assessment refers to a new or to an existing chemical or material. Generally, the available information for new chemicals and materials could be limited, thus a tiered approach will allow performing the hazard characterisation already in the innovation phase (i.e. during the design of the chemical or material) by using, for example, NAMs for data and knowledge generation (see the proposed approach in Section 6). Such a tiered approach will allow screening out suspected hazardous chemicals at an early stage in the innovation process and require data gradually along the life cycle. High-throughput screening, computer-based models, read-across and other non-animal approaches should be used so that only the most promising candidates (e.g. less hazardous) are tested on animals following the regulatory requirements for chemicals to be placed on the market. A screening of available independent (academic) data should also be done before deciding on the need for additional studies. However, any approach taken will require the definition of **minimum data (information) requirements** and establish the level of data needed to fulfil a criterion, which should not fall below the legal requirements defined in REACH.

Inclusion of data generated by NAMs (see *Section 6*) and screening for possible hazards properties at an early stage of the R&D process will allow also the assessment of chemicals not covered by REACH or other regulatory obligations. In this context it should also be noted that the hazard screening of any new chemical would use NAMs and only if the need arises would *in vivo* testing be performed, whereas existing chemicals would already have the regulatory relevant data associated.

In addition, the assessment approach and recommended methods for the list of hazard properties listed in Table 3 are included in the:

- ECHA Guidance on Information Requirements and Chemical Safety Assessment (ECHA, 2021b) that describes the information requirements and how to fulfil them under REACH regarding substance properties in the context of the chemical safety assessment
- ECHA Guidance on the Application of the CLP Criteria (ECHA, 2017a) that defines the criteria regarding the hazard properties.

These are supported by guidance documents, test guidelines/methods and recommendations on the implementation and on how to fulfil the regulatory requirements. In addition, the internationally recognised and accepted OECD Guidelines for the Testing of Chemicals (OECD, 2021) are one of the main tools for assessing the potential adverse effects of chemicals on human health and the environment. In the EU, the OECD test guidelines are taken up by the Test Methods Regulation that makes them legally binding in the EU (EU, 2008).

Criteria definition

The criteria refer to elements related to the intrinsic hazard properties of the chemicals or materials, relevant to physical hazards, the human health and the environment. The hazard-based criteria in the context of SSbD should ensure that the most harmful chemicals and materials, as defined by the criteria, are excluded already

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[23] Carcinogen means a substance or a mixture of substances which induce cancer or increase its incidence (Regulation (EC) No 1272/2008)

at the early R&D phase of developing new chemicals or materials, and that existing chemicals or materials having these properties are substituted. Also, implementing such criteria will support further aims, e.g. ensuring that products do not contain the most harmful substances (as defined in the CSS), that the substances of concern are substituted as far as possible and that a need for a new design (or redesign) for the chemical or material is identified.

Based on the hazard properties listed in Table 3, three criteria (H1, H2 and H3) were defined (Table 4) and a workflow was developed in order to integrate them (Figure 12). Several levels are established based on the fulfilment of these criteria. In addition, several elements need to be considered or further analysed, e.g.:

- The framework should be updated when new CLP criteria become available. Meanwhile, the inclusion of additional hazard criteria (e.g. soil and sediment toxicity) not yet covered by CLP should be further investigated in this context.
- Additional hazard endpoints (not covered by CLP) could be proposed to be added to the initial list of hazard properties in Table 3 (e.g. specific to particular materials, new biological endpoints) (*see Section 6 on NAMs data*).
- Material-specific criteria (e.g. considering morphology for nanomaterials, fibres) should be also developed, in addition to the general criteria.
- The Criteria H1-H3 are hierarchic, meaning that they need to be assessed one after the other, and the next criterion will only be assessed if the previous has been passed.
- If there is confirming evidence that the chemical or material possesses one of the hazard properties included in the criterion under evaluation, there is no need to gather information on the other properties from the same criterion. This aims to simplify the assessment and data gathering and eliminate problematic chemicals/materials faster, in an early stage of R&D process. However, in order to continue to the next criterion, evidence regarding all aspects that belong to the same set of criteria needs to be provided.

Table 4. Description of criteria related to Step 1

Criteria	Description	**Observations** (in alignment with CSS)
Criterion H1	The criterion refers to the **most harmful substances**, according to CSS, including the substances of very high concern (SVHC) according to REACH Art. 57(a-f) and additional hazard properties, as defined in Table 3. This is a cut-off criterion, establishing a minimum set of hazard requirements that need to be fulfilled by a chemical or material in order to be considered eventually SSbD after the other assessments are performed. Therefore, the assessment of the other aspects can be performed in order to understand the overall SSbD performance (e.g. safety during the use assessed in Step 3, other environmental sustainability aspects assessed in Step 4) if this helps the innovation process.	The chemicals and materials which do not pass this criterion should be: - Prioritised for substitution - Re-designed in order to reduce their adverse effects - Only allowed in uses proven essential for society (e.g. if their use is necessary for health, safety or is critical for the functioning of society and if there are no alternatives that are acceptable from the standpoint of environment and health)[24] - Safely used and emissions/exposure be controlled along the whole life cycle while activities are undertaken to develop alternatives as soon as possible and their use is phased out as soon as less hazardous alternatives are available - Tracked through their life cycle
Criterion H2	The criterion refers to the hazard class categories and hazardous substances which are part of the **substances of concern** described in CSS and not included already in criterion H1, as defined in Table 3. For the chemicals or materials with hazard properties a safety level or score will be assigned, while the SSbD assessment will continue with the evaluation of the other safety and sustainability aspects, in order to assess their overall SSbD performance.	The chemicals and materials that do not pass this criterion should be: - Substituted as far as possible - Re-designed in order to reduce their adverse effects - Safely used and emissions/exposure be controlled along the whole life cycle, until less hazardous alternatives are available - Tracked through their life cycle
Criterion H3	The criterion refers to the group of **other hazard classes**, including here all hazard properties not covered by criteria H1 and H2, as defined in Table 3. Following a similar approach described above, a safety level or score will be assigned to the chemicals or materials under this category in order to be integrated in the overall SSbD assessment.	The chemicals and materials that do not pass this criterion should be: - Flagged for review and eventually reduce toxic effects - Ensure their safety along the life cycle until less hazardous alternatives are available

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[24] Note that there are other initiatives of the EC under the CSS implementation that cover aspects such as Generic Risk Assessment, essential uses, etc.

Following the establishment of the top-level criteria described above, they could be broken down into sub-criteria that could cover detailed elements, e.g. assess separately the hazard properties relevant for human health or environment, score or weight individually the aspects that are currently grouped under the same criterion, include the methodology type applied for the hazard assessment (e.g. use of New Approach Methodologies versus *in vivo* testing). These sub-criteria could be defined, as needed, in the next phase of the framework development during the case studies exercise, as more information will be available.

In the next phase of the project, the proposed criteria will be tested, further developed, and refined during the case studies implementation. Their feasibility will be also evaluated.

Evaluation system

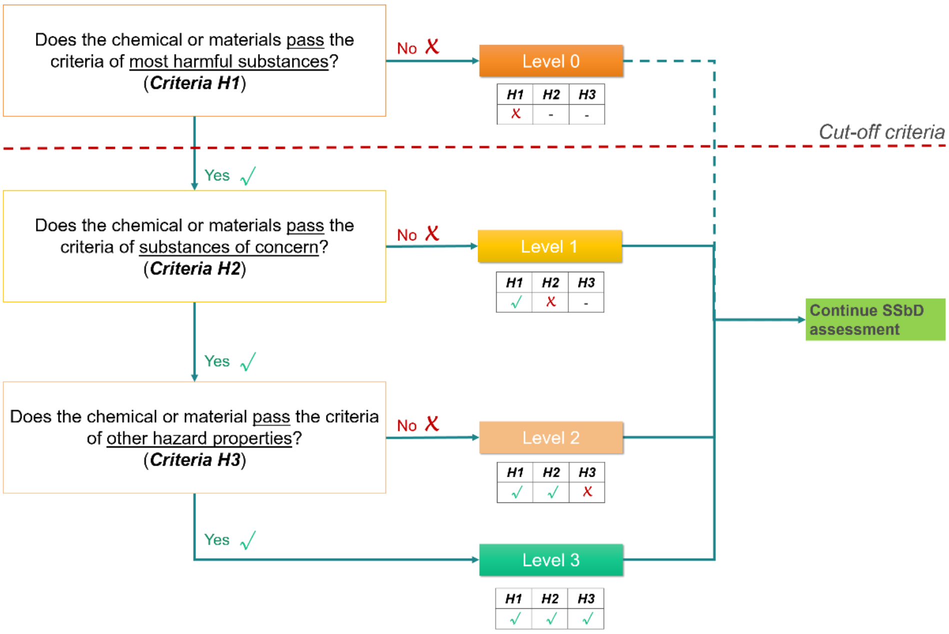
The chemicals or materials that pass a certain criterion of Step 1 will get a 'level' that reflects the result of the hazard assessment related to aspects included in that specific criterion.

For Step 1, four levels are currently envisioned (*from 'Level 0' to 'Level 3'*) that will allow the assessor to rank a specific chemical based on these levels and further to integrate the results of the hazard-based evaluation to the overall SSbD assessment (Figure 12):

- **Level 0** - chemicals or materials that do not pass hazard criterion H1 (e.g. considered most harmful substances)
- **Level 1** - chemicals or materials that pass hazard criterion H1 but do not pass criterion H2 (e.g. induce chronic effects, part of the substances of concern)
- **Level 2** - chemicals or materials that pass hazard criteria H1 and H2 but do not pass criterion H3 (e.g. with other hazard properties)
- **Level 3** - chemicals or materials that pass all safety criteria in Step 1. For Level 3 chemicals or materials that are considered to be of no concern regarding intrinsic hazard properties it should be recognised that the chemical/material could still pose harm in certain applications from a risk perspective that goes beyond generic hazard criteria and includes consideration of application-specific exposure settings.

Further, a detailed scoring system could be also developed for the safety Step 1 criteria, to give more detailed information regarding hazard properties evaluated and to support the decision of inclusion of a chemical or material into a particular level.

Figure 12. Workflow relevant to Step 1 of the SSbD framework



4.2.2 Human health and safety aspects in the chemical/material production and processing phase (Step 2)

This step evaluates the occupational safety and health (OSH) aspects in the life cycle of the chemical/material prior to its final application.

For this evaluation, it is important to identify all the production and processing steps, the chemicals used in each of them (raw chemicals/materials, processing aids…), the ones that may be produced during the processes (welding fumes, etc.), and identify their hazards.

The operational conditions (how the substance is used, duration, concentration in a preparation, outdoor/indoor use, close/open process) together with the potential of release (Volatility, dustiness, fugacity, temperature, pressure) and the Risk Management Measures (RMMs) in place (e.g. Local Exhaust Ventilation) will identify the likelihood of the exposure to the chemical/material as well as the potential route (inhalation, dermal, ingestion) of exposure.

The methodology includes the following:

- Definition of the aspects and indicators to be included
- Definition of criteria
- Evaluation system

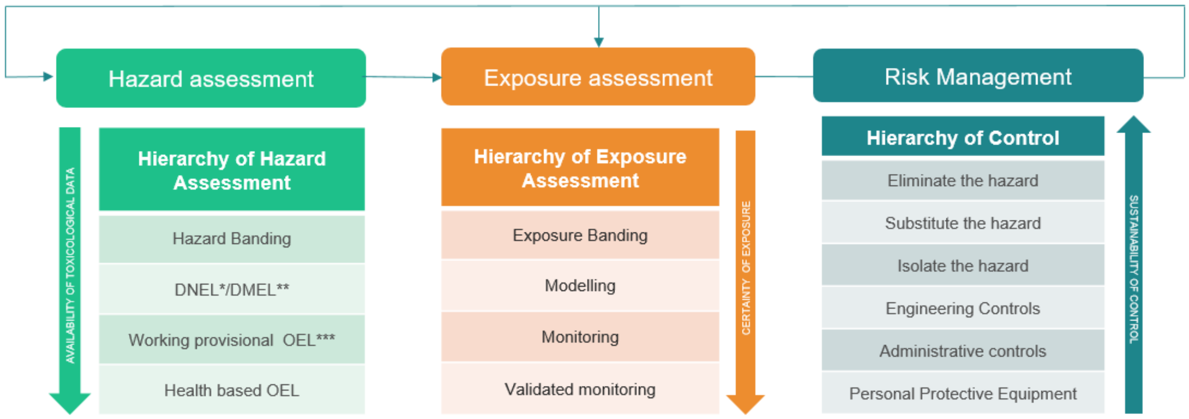
Aspects and indicators

The aspects to be included in this Step will be the ones related to the human health and safety during the production and processing of chemical/material. The risk should be estimated as a combination of the chemical/material hazards and the exposure during the different processes process and the RMMs already in place to control the risks.

As in Step 1, a tiered approach can be applied, depending on whether the assessment refers to a new or to an existing chemical or material and the availability of the data in the different cases.

Figure 13 illustrates a hierarchy for tiered risk assessment depending on the data availability for each of the aspects.

Figure 13. Hierarchy for a tiered risk assessment depending on the data availability for each of the aspects (Laszcz-Davis et al., 2014)



*Derived No Effect Level
**Derived Minimum Effect Level
***Occupation Exposure Limit

There are different qualitative/simplified models available (also known control banding models) for the safety assessment and management at the workplace. These models are designed to characterise the risk at the workplace in a Tier 1 approach, when the whole set of data to perform a quantitative assessment is not available. These models are based on assigning scores or levels to some of the following variables to be taken into account during the risk characterisation:

- Hazards of chemicals
- Exposure frequency and duration
- Amount of chemical used or present
- Physical properties of the chemical like volatility and dustiness
- Operational conditions
- Type of existing RMMs
- Others

The result is a categorisation into different risk levels, which determine whether the risk is acceptable or not, and sometimes, the type of preventive measures to be applied.

There are two types of models: those that estimate the potential risk of exposure (they do not include the preventive measures taken as an input variable) and those that estimate the expected risk of exposure (they estimate the final risk considering the measures already implemented, if any).

These models were originally developed by the pharmaceutical industry as a way to safely work with new chemicals that had little or no toxicity information and in 1999 the first general model, COSHH Essentials[25], was published by the British Institute of Occupational Safety (Health and Safety Executive, HSE). Since then, new tools have emerged based on the same approach (ILO model[26] and the German Hazardous Substances (GHS) Column Model (see Annex 3) supported by the 'Easy-to-use Workplace Control Scheme for Hazardous Substances' (EMKG) tool[27]), from a different approach (INRS model[28]) or by expanding the complexity or combining both approaches (Dutch Stoffenmanager model[29] and Belgian REGETOX model[30]).

A more complex but still qualitative tool that could be used in this Step is the tiered Targeted Risk Assessment (TRA) tool[31] developed by ECETOC (The European Centre for Ecotoxicology and Toxicology of Chemicals). ECETOC TRA was developed with the aim of aiding the registration of chemicals under REACH and is widely used by industry and known by SMEs (Wijnhoven and Affourtit, 2018). In order to use this tool, it is recommended to apply the ECHA guidance Chapter R12 Use description to define the use of the chemical/material in the different stages since the tool uses this guidance as a reference (ECHA, 2015).

Chesar[32] is another tool recommended for the safety assessment of the chemical/material. The tool was developed by ECHA for assisting companies in producing chemical safety reports (CSR) and exposure scenarios (ES). It contains the ECETOC TRA plugin for the consumer exposure estimate and also contains support for environmental exposure estimates with the EUSES 2.1[33] fate model, and a release module to estimate environmental releases and the corresponding conditions of use. The release estimates are related to classes on emission characteristics, known as Environmental Release Categories (ERCs) also provided in the R12 guidance, release factors or Specific Environmental Release Categories (SpERCs). SpERCs are part of the use maps developed by industry sectors collecting information on the uses and the conditions of use of chemicals in their sector in a harmonised and structured way. Chesar also provides a library of use maps that can be used in the chemical/material safety assessment. This library includes the use description and the input parameters for workers exposure assessment (SWEDs), for consumers exposure assessment (SCEDs) and for environmental exposure assessment (SPERCs).

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[25] Control of Substances Hazardous to Health (COSHH) https://www.hse.gov.uk/coshh/essentials/index.htm

[26] International Labour Organization - International Chemical Control Toolkit https://www.ilo.org/legacy/english/protection/safework/ctrl_banding/toolkit/icct/

[27] Easy-to-use Workplace Control Scheme for Hazardous Substances (EMKG) https://www.baua.de/EN/Topics/Work-design/Hazardous-substances/EMKG/Easy-to-use-workplace-control-scheme-EMKG_node.html

[28] INRS model https://www.inrs.fr/media.html?refINRS=ND%202233

[29] Stoffenmanager https://stoffenmanager.com/en/

[30] REseau de GEstion des risques TOXicologiques (REGETOX 2000) http://www.regetox.med.ulg.ac.be/accueil_fr.htm

[31] ECETOC's Targeted Risk Assessment (TRA) tool https://www.ecetoc.org/tools/tra-main/

[32] CHEmical Safety Assessment and Reporting tool https://chesar.echa.europa.eu/home

[33] European Union System for the Evaluation of Substances https://echa.europa.eu/support/dossier-submission-tools/euses

Criteria definition

From the aspects to be considered in Step 2, a set of criteria can be defined in order to assess the hazard and exposure aspects to estimate the risks from all the processes along the life cycle. The criteria will address the use of hazardous chemicals/materials as well as the process related potential of exposure.

The application of such criteria will give additional information on the worker safety in the different processes along the life cycle (e.g. extraction, production, recycling, waste treatment) that will contribute to the overall sustainability indicators.

As for the Step 1, once the main set of criteria are established, each could contain several sub-criteria to be defined, as needed during the case studies implementation.

Another option to be evaluated, is whether the criteria can be applied to any step during the production and processing or more specific criteria should be developed for each of them.

Evaluation system

Once criteria are defined, a score can be attributed to each of them from 1 = very high-risk to 5= negligible risk, as shown as an example in Table 5.

Table 5. Example of a scoring system proposed for Step 2

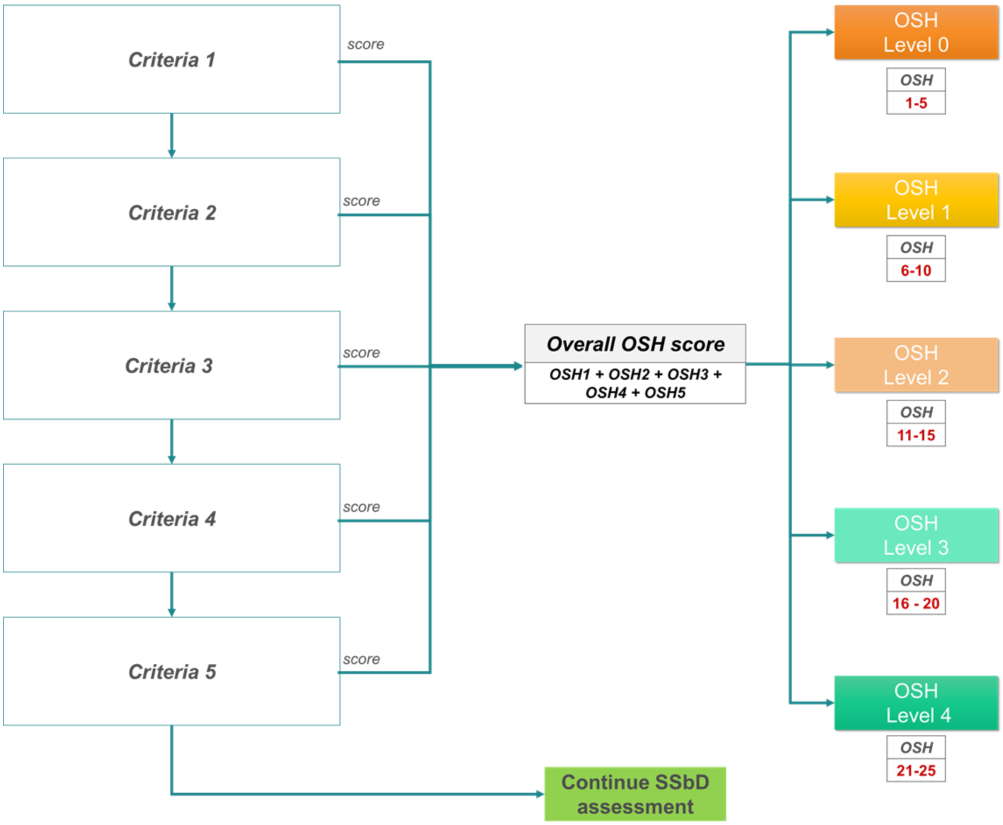
Criteria 1	Criteria 2	Criteria 3	Criteria 4	Criteria 5	Safety	
4	4	5	5	5	21-25	Negligible risk
3	3	4	4	5	16-20	Low-risk
1	2	3	3	4	11-15	Medium-risk
1	1	2	2	3	6-10	High-risk
1	1	1	1	1	0-5	Very high risk

The sum of the scores for each aspect will represent the overall OSH score (min 1 and max 25, if each aspect has the same weight in the final result) that will show the process safety level (from very high-risk process to negligible risk of the process), e.g.:

- OSH Level 0 = Very high risk process (overall score 1-5)
- OSH Level 1 = High risk process (overall score 6-10)
- OSH Level 2 = Medium risk process (overall score 11-15)
- OSH Level 3 = Low risk process (overall score 16-20)
- OSH Level 4 = Negligible risk process (overall score 21-25)

The OSH score will be reflected in the overall SSbD level. The workflow related to this step is shown in Figure 14. Further refinements of Step 2 evaluation system could address for example the different weighting of the aspects included, establishment of pass / fail criteria, etc.

Figure 14. Workflow relevant to Step 2 of the SSbD framework



4.2.3 Human health and environmental aspects in the final application phase (Step 3)

This step evaluates the human and environmental aspects in the application of the chemical/material. Similar to Step 2, the conditions of use will identify the likelihood of the exposure to the chemical/material as well as the potential routes of exposure (all relevant pathways) and the related toxicity impacts for the human health, including service-life exposure and the environment (e.g. from wash-off uses, like shampoo ending up in wastewater treatment plant effluents).

The methodology includes the following:

- Definition of the aspects and indicators to be included
- Definition of criteria
- Evaluation system

Aspects and Indicators

The aspects to be included in this Step will be the ones related to the human health and environment during the application of the chemical/material. The risk is characterised as a combination of the chemical/material hazards and the exposure assessment to the human health and the environment during the application. Figure 15 provides the workflow for the assessment the aspects.

Therefore, information on the substance/material's intrinsic properties are necessary for the safety assessment. This mainly concerns to the intrinsic properties for the hazard assessment in Step 1: Physical hazards, environmental hazards and human health hazards.

Other physical-chemical properties are also needed to identify the fate of the chemical/material, estimate the exposure path and characterise the risk. Properties like the physical form and vapour pressure for the human health and the water solubility and octanol water partition coefficient (Log Kow) for the environment.

For the exposure estimation, it is particularly important to identify/describe the application and define the use conditions providing information on, frequency and duration of the exposure, amount of chemical/material used or present in the application, use conditions and use instructions.

As in previous steps, depending on whether the assessment refers to a new or to an existing chemical/material, and the availability of the data, the approach might be different.

As in Step 2, it is also recommended to apply the ECHA guidance (R12 Use description) to define the application in this step. R.12 guidance provides lists of Product Categories (PCs) and Article Categories (ACs) and many available exposure estimation tools like ECETOC TRA use these use description categories as input elements for the exposure and safety assessment.

Chesar is another tool recommended for the safety assessment of the chemical/material. The tool was developed by ECHA for assisting companies in producing chemical safety reports (CSR) and exposure scenarios (ES). It contains the ECETOC TRA plugin for the consumer exposure estimate and also contains support for environmental exposure estimates with the EUSES 2.1 fate model, and a release module to estimate environmental releases and the corresponding conditions of use. The release estimates are related to classes on emission characteristics, known as Environmental Release Categories (ERCs) also provided in the R12 guidance, release factors or Specific Environmental Release Categories (SpERCs). SpERCs are part of the use maps developed by industry sectors collecting information on the uses and the conditions of use of chemicals in their sector in a harmonised and structured way. Chesar also provides a library of use maps that can be used in the chemical/material safety assessment. This library includes the use description and the input parameters for workers exposure assessment (SWEDs), for consumers' exposure assessment (SCEDs) and for environmental exposure assessment (SPERCs).

As in Step 2, higher Tier tools, expanding the complexity, can also be used when data availability allows it like for example ConsExpo or the tools developed by industry sectors for the assessment of specific product types and articles.

During the case studies, it is also foreseen to apply life cycle-oriented tools like ProScale 1.5 (Lexén et al., 2017) and USEtox[34] in order to compare them both from the feasibility and applicability point of view, including the need for data etcetera, and from a point of view of the validity and usefulness of results. ProScale is explicitly based on ECETOC TRA while USEtox 3 is based on Global Guidance for Life Cycle Impact Assessment Indicators and Methods (GLAM)[35] recommendations, which are based on earlier WHO consensus in risk assessment to derive human toxicity effects. The USEtox 3 approach combines intake fractions (for emissions from e.g. processes) and product intake fractions (for chemicals/materials in product applications) as exposure metric and combine it with effect factors. ProScale and USEtox are both methods developed in the context of the life cycle assessment to characterise human and environmental impacts of chemicals /materials through the entire life cycle. USEtox 3 explicitly also includes reference doses etc. for application in chemical substitution and risk screening. Beyond Step 3 itself, these methods also serve as a link to Step 4.

Definition of criteria

A set of criteria can be defined to assess the human health and environment aspects. The application of such criteria will give additional information on the consumer and environment safety during the use that will contribute to the overall sustainability indicators.

As for the Step 1 and Step 2 once the main set of criteria are established, each could contain several sub-criteria to be defined, as needed during the case studies implementation. Another option to be evaluated is

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[34] USEtox 3 https://usetox.org/model/download/usetox-3.0beta

[35] Global Guidance for Life Cycle Impact Assessment Indicators and Methods (GLAM) https://www.lifecycleinitiative.org/activities/key-programme-areas/life-cycle-knowledge-consensus-and-platform/global-guidance-for-life-cycle-impact-assessment-indicators-and-methods-glam/

whether the criteria can be applied to any application or more specific criteria should be developed for different applications.

Evaluation system

Once criteria are defined different safety levels can be defined both for the human health and the environment and a score and a colour code can be assigned to determine whether the criterion is considered as ‘passed’ or not, as in the example in Table 6.

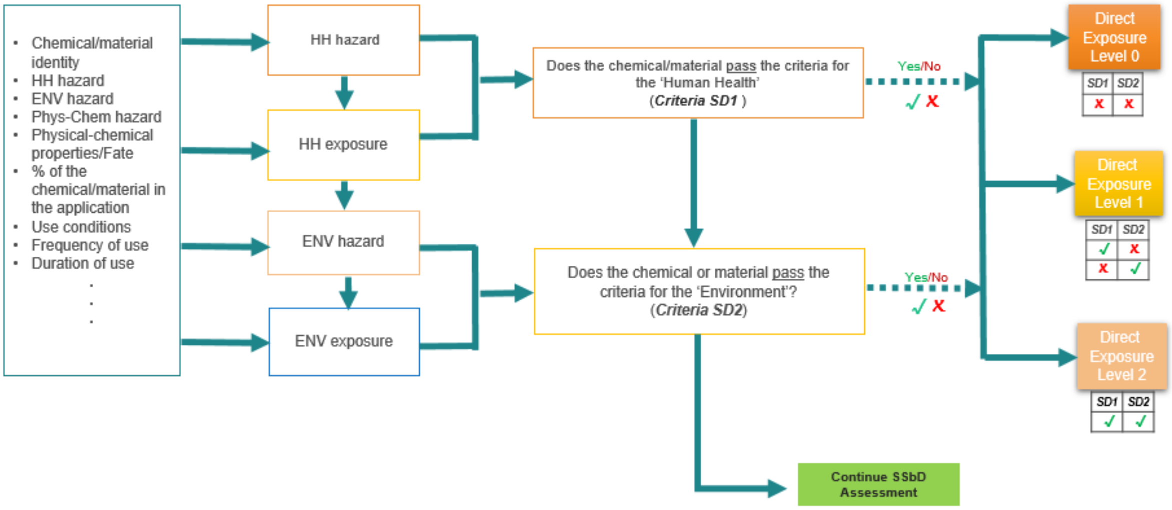
Table 6. Scores to be applied for each aspect. Note that these ‘classes” are illustrative and should be defined considering the uncertainty of the assessment.

Position to safe level	Score	Colour code	Criteria evaluation
> Safe level + 50%	0	🟥	Fail the criteria
>Safe level; < safe level +50%	1	🟧	
>Safe level - 25% ; < Safe level	2	🟨	Pass the criteria
>safe level -50% ; <Safe level - 25%	3	🟩	
< Safe level – 50%	4	🟦	

And as illustrated in Figure 15, the combination of the human health and environment safety will provide the overall safety in the application phase.

- Level 0: The chemical/material fails to pass both criteria
- Level 1: One of the two criteria is passes by the chemical/material
- Level 2: The chemical/material passes both criteria

Figure 15. Workflow relevant to Step3 Human health and environmental effects in the application use phase of the SSbD framework. Please note that this scheme refers to steps to be followed and is not entailing exclusion criteria.



4.2.4 Environmental sustainability assessment (Step 4)

This step covers the assessment of the environmental sustainability aspects of the chemical or material, with a specific focus on environmental impacts along the entire value chain, from extraction of raw materials up to waste management. As mentioned previously, the EU CSS calls for the development of SSbD criteria for chemicals to be defined through a holistic framework integrating the minimisation of the environmental footprint of chemicals with their safety, circularity, and functionality throughout their entire lifecycle. Life cycle assessment is then proposed as a method to assess the environmental impacts of chemical production, use and end of life.

As mentioned previously, the environmental sustainability is associated with an absolute sustainability assessment, so that the impacts of chemical/material and its production system(s) are within planetary boundaries. This assessment corresponds to the high level of ambition in the CSS, and current proposed methods aim at exploring and testing feasibility of absolute sustainability assessment.

Moreover, the deliberation if a chemical/material is SSbD can only be done if the intended use(s) is considered. Therefore, to assess the environmental sustainability of the chemical/ material, a function-based LCA including the entire life cycle must be conducted. If the new chemical/material has several possible uses, or if it can be produced via several production routes, different LCAs must be conducted considering each use as well as its respective end of life. Aspects related to boundary conditions, foundation for comparison or function level, multi-functional chemicals, or materials, etc. need to be considered. The LCA studies should be conducted following the same modelling principles to ensure its harmonisation and allow comparison of results. Box 1 presents a brief overview of LCA guidelines as well as current limitations regarding its use in the context of SSbD. In any case, the LCA results must be presented stating clearly the assumptions and data sources used.

Box 1. LCA modelling guidance

LCA modelling guidance in the context of SSbD

To ensure the comparability of LCA studies that are used in the SSbD context specific guidance should be developed.

In the meanwhile, it is recommended to refer to existing EC guidelines, i.e. the Product Environmental Footprint (PEF) method (EC, 2021f), which is the European Commission recommended method to assess the life cycle environmental performance of products on the market (EC, 2021f). The method is inspired by the ISO 14040 and 14044 (ISO, 2006, ISO, 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).

It is also common practice in LCA frameworks to develop specific rules for categories of similar products in order to provide more guidance related to the specificity related to the life cycle of that products (e.g. primary data required, specific allocation rules for multi-functional processes, secondary data to be used). In the context of the PEF, these rules are called Product Environmental Footprint Category Rules (PEFCR). Currently, there are no PEFCRs specifically addressing chemicals. Guidance on the LCA of chemicals and materials can be found in the "Life Cycle metrics for Chemical Products" (WBCSD, 2014) or in scientific literature (Fantke and Ernstoff, 2018, Maranghi and Brondi 2020).

To conduct a LCA in the SSbD context entails specific challenges such as the low TRL of the technologies. When the maturity level of a technology is low (e.g., TRL <5), it is usually difficult to perform a proper LCA due to low representativeness of primary data (e.g., data from lab scale pilot differ from real industrial plant data). To overcome this issue in the latest years there is a growing interest in Prospective LCA, that aim to provide guidance on extrapolation of meaningful inventory data for LCA from lab/pilot processes to industrial scale. On this topic, see the work from Ardvisson et al. 2017, Cucurachi et al. 2018, van der Giesen et al. 2020, van der Hulst et al. 2020.

Another relevant aspect addressed by the prospective LCA is how to model product systems considering the evolution of the industrial context and emerging technologies (e.g., the shift of energy systems toward higher share of renewables or reduction of environmental imapcts), which can be useful for the SSbD to understand how environmental impacts of chemicals can change as a consequence of changes in the industrial environment (Sacchi et al. 2022).

In the following sections, we describe:

- Which aspects and indicators to consider
- Definition of criteria
- Evaluation system

Aspects and indicators to be considered

Environmental sustainability embraces a variety of different aspects (see e.g. the taxonomy of impacts proposed by Bare and Gloria, 2008). Some aspects are widely modelled, such as the impact categories considered in the Environmental Footprint Impact assessment method with the respective indicators. This method is recommended by the European Commission to be used to assess the life cycle environmental performance of products (EC, 2021f) and could be considered as a minimum set of impacts to be addressed when conducting an LCA study. Other aspects are not yet fully covered by current LCA practices and might need to be addressed on a case-by-case basis by the criteria developer, addressing possible indicators and ranges.

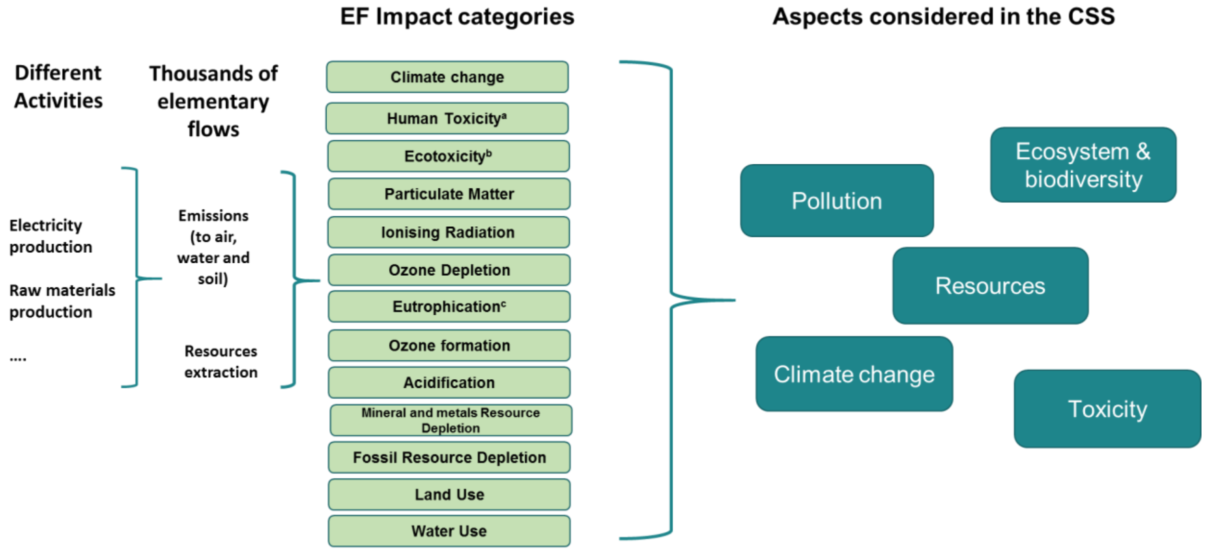
Regarding the Environmental footprint, as illustrated in **Figure 16**, the method considers in total 16 impact categories that are related to several policy objectives such as protection of human health and of biodiversity. It is important to note that in the real world the different environmental aspects are interlinked as, for example, pollution and climate change are key drivers of impacts on biodiversity loss and human health. The method includes human toxicity (cancer and non-cancer) and ecotoxicity impact categories that relate to the main goal of SSbD, which is to use only chemicals that help moving towards a 'toxic-free environment'. These impact categories differ from the assessment conducted in Step 3 as they 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 assessment is rather on indirect impacts via different compartments and in the overall toxicity footprint rather than a specific focus on direct exposure. These toxicity related impact categories rely on a multimedia box model, i.e. address also the transfer of chemicals from one compartment to the other due to the specific physico chemical properties of the chemicals which are assessed.

Aside the 3 impacts categories related to toxicity, the method includes other 13 impact categories, providing a broader view on the environmental performance of the chemical/material. The 16 impacts categories relate to the CSS objective of minimising the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity (Figure 16).

The 16 impact categories (see Table 7) are result from modelling of 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) by the impact characterisation factors associated to each of them (by means of coefficients/characterisation factors which attribute an impact score to each elementary flows). The 16 indicators could be expressed also as a single score. However, we suggest retaining the 16 individual indicators for reporting to better illustrate the trade-offs among them and the main hotspots.

We propose to cluster the different impacts categories in 4 groups: toxicity, climate change, pollution, and resources, as presented in Table 7, reflecting LCA assessment levels that relate to the different policy objectives. Currently, there is not an impact category in the EF method addressing biodiversity loss. Nevertheless, the EF method account for the main drivers for biodiversity loss such as Climate Change or Land Use. Hence, EF results could be considered a proxy of biodiversity footprint by means of the underpinning drivers of loss. Moreover, in operational LCA frameworks, "functional diversity" and related "ecosystem services" assessment methods are currently not included, and underlying models for several impact categories not yet fully operational (e.g. ecotoxicity in EF focuses on freshwater organisms only., whereas a complete ecotoxicity assessment would need to address on terrestrial, marine, soil, and sediment organisms as well.

Figure 16. Environmental Footprint (EF) impact categories related to issues considered in the Chemicals Strategy (CSS)



^{a} two impact categories: cancer and non-cancer; ^{b} freshwater; ^{c} three impact categories: terrestrial, freshwater, and marine eutrophication

It is important to note that toxicity impacts categories also relate to pollution. Nevertheless, we opted by having a separate group for the toxicity impacts categories in this step as they are related with aspects covered in the previous steps. This will allow us to identify any overlapping among the steps when conducting the case-studies, during which a detailed analysis of the underpinning data used in each step will be done. A short description of each impact category covered in the EF method is provided in Annex 4.

Acknowledging that the existing environmental impacts go beyond those covered in the EF method (Bare and Gloria, 2008) we leave open the addition of other impact categories and related criteria could be proposed and included. Also, several life cycle impact assessment (LCIA) methods to assess impacts on biodiversity exist (e.g. 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.

Table 7. Recommended models for the Environmental Footprint method including indicator, units and models[36]

LCA Assessment level	**Impact category**	**Indicator**	**Unit**	**Recommended default LCIA model**
Toxicity	**Human toxicity, cancer effects**	Comparative Toxic Unit for humans (CTU_h)	CTUh	based on USEtox2.1 model (Fantke et al., 2017) adapted as in (Saouter et al., 2018)
	Human toxicity, non-cancer effects	Comparative Toxic Unit for humans (CTU_h)	CTUh	based on USEtox2.1 model (Fantke et al. 2017), adapted as in Saouter et al., 2018)

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[36] LCIA models are subjects to further refinements. To access the most updated list of models and indicators, the reader is invited to consult the list published in the European platform on life cycle assessment (https://eplca.jrc.ec.europa.eu/)

LCA Assessment level	Impact category	Indicator	Unit	Recommended default LCIA model
	Ecotoxicity freshwater	Comparative Toxic Unit for ecosystems (CTU_e)	CTUe	based on USEtox2.1 model (Fantke et al. 2017), adapted as in Saouter et al., 2018)
Climate Change	**Climate change**	Global warming potential (GWP100)	kg CO_2 eq	Bern model - Global warming potentials (GWP) over a 100-year time horizon (based on (IPCC, 2013)
Pollution	**Ozone depletion**	Ozone Depletion Potential (ODP)	kg CFC-11eq	EDIP model based on the ODPs of the World Meteorological Organisation (WMO) over an infinite time horizon ((WMO, 2014)+ integrations)
	Particulate matter/Respiratory inorganics	Human health effects associated with exposure to $PM_{2.5}$	Disease incidences[37]	PM model (Fantke et al., 2016) in (UNEP, 2016)
	Ionising radiation, human health	Human exposure to ^{235}U	kBq ^{235}U	Human health effect model as developed by Dreicer et al., 1995 (Frischknecht et al, 2000)
	Photochemical ozone formation	Tropospheric ozone concentration increase	kg NMVOC eq	LOTOS-EUROS (Van Zelm et al., 2008) as applied in ReCiPe 2008
	Acidification	Accumulated Exceedance (AE)	mol H+ eq	Accumulated Exceedance (Posch et al., 2008; Seppälä, et al., 2006)
	Eutrophication, terrestrial	Accumulated Exceedance (AE)	mol N eq	Accumulated Exceedance (Seppälä et al. 2006, Posch et al, 2008)
	Eutrophication, aquatic freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P eq	EUTREND model (Struijs, et al. 2009)as implemented in ReCiPe 2008
	Eutrophication, aquatic marine	Fraction of nutrients reaching marine end compartment (N)	kg N eq	EUTREND model (Struijs et al, 2009) as implemented in ReCiPe 2008
Resources	**Land use**	Soil quality index[38] aggregating: Biotic production, Erosion resistance, Mechanical filtration and Groundwater replenishment	Dimensionless*	Soil quality index based on LANCA model (De Laurentiis et al., 2019) and on the LANCA CF version 2.5 (Horn and Maier, 2018)
	Water use	User deprivation potential (deprivation weighted water consumption)	m^3 water eq of deprived water	Available WAter REmaining (AWARE) model (Boulay et al., 2018; UNEP, 2016)
	Resource use, minerals and metals	Abiotic resource depletion (ADP ultimate reserves)	kg Sb eq	CML (Guinée et al., 2002) and (Van Oers et al. 2002)
	Resource use, energy carriers	Abiotic resource depletion – fossil fuels (ADP-fossil)[39]	MJ	CML (Guinée et al., 2002) and (Van Oers et al. 2002)

*dimensionless index[40] resulting from the aggregation of the individual indicators for soil covering: biotic production (kg biotic production/ (m^2*a)); Erosion resistance (kg soil/ (m^2*a)); mechanical filtration (m^3 water/ (m^2*a)); and groundwater replenishment (m^3 groundwater/ (m^2*a)).

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[37] The name of the unit is changed from “Deaths” in the original source (UNEP, 2016) to “Disease incidences”

[38] This index is the result of the aggregation, performed by JRC, of the 4 indicators provided by LANCA model for assessing impacts due to land use as reported in De Laurentiis et al, (2019).

[39] In the ILCD flow list, and for the current recommendation, Uranium is included in the list of energy carriers, and it is measured in MJ.

[40] This refers to both land occupation and transformation

Definition of criteria

For each impact category a criterion should be defined as a **reduction of the impact category value of X% (target) relative to a reference value.** There is, therefore, the need to define the reduction factor (X) and the reference. Ideally, existing criteria defined in other initiatives such as Ecolabel, EU ETS, and Sustainable Finance should be taken into consideration when developing criteria for SSbD chemicals and materials.

As observed in the literature reviewed, several frameworks and approaches exist that allow to compare alternative chemicals, thus guiding relative improvement on the safety and sustainability of chemicals (despite the latter being often limited to few environmental indicators). The ambition of the SSbD is to move from relative (safer and more sustainable) to absolute (safe and sustainable) improvements ensuring that chemicals and materials are produced and used without exceeding acceptable boundaries. Therefore, targets should be defined according to this. Setting such a science-based target requires:

- a global (or regional, depending on the impact being considered) assessment of the current magnitude of a problem and its future trajectories;
- building a consensus on the acceptable level of impact that society can tolerate.

The difference between the magnitude of the problem (current impact) and a consensus on the acceptable level of impacts can be used as the target for reduction that can then be scaled down to the chemical/material.

For example, Global assessments in other fields such as IPCC's (Intergovernmental Panel on Climate Change) Assessment Reports[41], the Global Burden of Disease studies[42] or the UN treaty on plastic pollution[43], have been instrumental in raising awareness and mobilising policy actions towards resolving the problems that they addressed. Currently, comprehensive assessments of the impacts of chemicals are scarce. Such an assessment would need to resolve not only data challenges but also some of the known methodological issues in subjects such as fate, transport and exposure modelling and aggregation of local and regional impacts, obtaining figures at relevant spatiotemporal scales. Ideally, a global/regional assessment of chemicals should be able to estimate the magnitude of impacts posed by chemicals in all areas of concern including:

- human morbidity and mortality from chemical exposure;
- biodiversity losses from chemical exposure;
- other environmental impacts associated with the life cycle of chemicals e.g. climate change, ozone layer depletion, eutrophication, acidification, resource depletion, water consumption.

The integration of ecosystems carrying capacities in environmental assessments has been advocated since long in the sustainability science domain (Sala et al., 2013a, b), and as a mean to move LCA from comparative to absolute assessment, leading to the development of LCA-based methods for Absolute Environmental Sustainability Assessment (AESA) (Bjørn et al. 2020).

The review carried out by Bjørn et al. (2020) presents an overview of the different LCA-based methods for AESA. According to the authors, the estimation of the environmental impacts can be done according to impact categories from the LCIA framework or the earth-system processed from the Planetary Boundary concept.

The Planetary Boundary (PB) framework, originally from Rockström et al. (2009a) and updated by Steffen et al. (2015), has proven to be an influential concept regarding the Earth's limited carrying capacity, i.e. natural capital cannot be unlimitedly exploited (Downing et al., 2019). The PB framework defines nine biophysical processes fundamental to Earth system functioning and define together a safe space for humans to act within while staying at a 'safe distance' from a tipping point or threshold. The PBs are expressed by so-called 'control variables' (CV) which are defined as environmental states or flow rates, such as atmospheric CO2 concentrations for climate change (Ryberg et al., 2018). The Safe Operating Space (SOS) is the difference between the PB and

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[41] https://www.ipcc.ch/reports/

[42] https://www.thelancet.com/gbd

[43] https://www.unep.org/news-and-stories/story/what-you-need-know-about-plastic-pollution-resolution

the natural occurring background level (NBL; usually representing pre-industrial conditions), thus indicating the maximum anthropogenic effects we can permit ourselves without destabilising Earth's systems (Rockström et al., 2009a). The nine planetary boundaries include: Climate Change, Biosphere Integrity, Stratospheric Ozone Depletion, Ocean Acidification, Biochemical Flows, Land-system change, Freshwater use, Atmospheric aerosol loading, and Novel Entities. In Annex 5 the nine planetary boundaries are presented. The PB 'novel entities' boundary (previously called 'chemical pollution' (Rockström et al., 2009b) is not yet defined. In recent years, different approaches have been explored (Diamond et al., 2015; Kosnik et al., 2022; Persson et al., 2022; Plaza-Hernández et al., 2021; Villarrubia-Gómez et al., 2018).

In the context of the SSbD, it is important to consider that "novel entities", including chemicals and plastic, are acknowledged as having their own PB and strictly link to toxic chemicals and their related life cycle emissions of other toxic chemicals. Other planetary boundaries (e.g. for "climate change") are also affected by emissions along chemical and material life cycles that are associated with flows other than toxic chemicals. For the specific case of boundaries/reference targets for chemical pollution (as compared to other boundaries, such as climate change), the spatial scale is of utmost importance as chemicals or materials are rarely as such planetary-scale problems, but cause transgression of local-to-regional boundaries in most cases (Kosnik et al. 2022). Regardless of these limitations and acknowledging that absolute environmental sustainability assessment is still an open challenge, the PB-framework offers a strong concept to understand and respect the biophysical limits of the Earth and could in the end support policy making when related to sustainability.

In recent years, several methods have been developed linking the PB-framework to LCA. There is, however, currently no common framework (Bjørn et al., 2019). In the past, weighting factors were developed to be used in the weighting step (Tuomisto et al., 2012; Vargas-Gonzalez et al., 2019), carrying capacity-based normalisation references for different midpoint categories (Bjørn and Hauschild, 2015; Sala et al., 2020; Uusitalo et al., 2019) and approaches to link the Safe Operating Space (SOS) to the Life Cycle Inventory (LCI) (Fang and Heijungs, 2014; Ryberg et al., 2016). Recently a comprehensive method was developed by Ryberg et al. (2018) proposing PB-informed characterisation models defining characterisation factors (CFs) to map the elementary flows onto the control variables. This method offers the opportunity of scaling the assessed activity after the impacts are expressed in PB metrics (Ryberg et al., 2018) and seems to be increasingly applied (Algunaibet et al., 2019; D'Angelo et al., 2021; Galán-Martín et al., 2021; Ryberg et al., 2021; Tulus et al., 2021; Valente et al., 2021). However, a key challenge in the application of this method is to determine the allocation of the SOS to the chemical/material under assessment. The case studies development will allow to explore and test some of these approaches and its application in the context of the SSbD.

Yet in the context of absolute sustainability, studies on the environmental impacts of EU production and consumption have shown that current level of impacts is 10 times higher than the acceptable limits, e.g. for climate change (Sala, et al. 2020). Since at the moment this information is not available for other impacts categories, this factor can be adopted as default and used to flag the impact categories in which most of the reduction is possible. This factor 10 is also referenced since long time as a mean for society to achieve sustainability (Schmidt-Bleek, 2008; Srinivas, 2015). Factor 10 states that over the next 30 to 50 years (one or two generations) a decrease in energy use and material flows by a factor of 10 and an increase in resource productivity/efficiency by a factor of 10 is required to achieve dematerialisation. That is, to attain sustainability and environmental protection we need to reduce resource turn over by 90% on a global scale, within the next 50 years.

Alternatively, one can adopt the proposed targets in EU policies such as that for Climate Change of 50% reduction or even carbon neutral.

Another possibility, to support the criteria development and define possible targets, is to use information in Best Available Techniques Reference (BREFs), which are a series of reference documents covering, as far as is practicable, the industrial activities listed in Annex 2 to the EU's IPCC Directive, providing descriptions of a range of industrial processes (for those that are available) and for example, their respective operating conditions and emission rates.

If one sets a factor 10 or 50% reduction, this should be done in relation to a reference. The reference should be defined ideally as the state of the art of the intended use. A possibility is the definition of a representative chemical/material within a chemical/material class or group that fulfil the same function. However, this could be particularly challenging in terms of granularity of the chemical class to be addressed, and when alternatives are proposed pertaining to different classes. Nevertheless, for some classes e.g. solvents rankings already exist so one should expand on these general lists and not fall below this standard by intentionally selecting worse reference chemicals/materials. So, criteria may result from collecting evidence of a significantly better environmental performance of the alternative compared to the base case.

A pragmatic approach is to compare the chemical/material under assessment with the incumbent chemical/material or among the possible alternatives in the design stage following what is done currently in alternative assessment. Despite easy to implement, this will lead only to relative improvements as the incumbent chemical/material might have a poor performance and therefore, even if performing better than the incumbent chemical/material the new chemical/material might be aligned with the ambitions of the SSbD concept set in this framework.

Evaluation system

Once the criteria for each impact category are defined one can assess the chemical/material attributing a score as illustrated (for example) in Table 8. For example, if the chemical/material shows no improvement relatively to the reference it would score 0, instead if the improvement is higher than 40% it would score 4. Note that these 'classes" are illustrative and should be defined considering the uncertainty of the assessment (both inventories and impacts assessment methods used). This will be further developed with the application of the framework to the case-studies. An illustrative example of the result of the evaluation is presented in Table 9.

Table 8. Scores to be applied for each impact category. Note that these 'classes" are illustrative and should be defined considering the uncertainty of the assessment

Position to reference	Score	Colour code	
No improvement	0	🟥	Fail the criteria
Improvement + 5%	1	🟧	
Improvement + 5% to 20%	2	🟨	Pass the criteria
Improvement + 20% to 40%	3	🟩	
Improvement > 40%	4	🟦	

The chemical/material that pass a certain criterion will get a 'level'. As illustrated in Figure 17 a 'LCA level' can be derived counting the number of passed assessment levels, being each level composed by different groups of impacts category as exemplified in Table 9 for the current EF impacts categories (which are grouped in 4 levels). A level is considered achieved if the chemical/material passes the criteria defined for all impact category in that level. Considering the example of Figure 17, the chemical/material can achieve a LCA level ranging from 0 (meaning that the chemical/material did not pass any of the assessment levels) to level 5 (meaning that the chemical/material passed all the assessment level). Note that level 5 is used here as a placeholder for additional aspects that could be included in the assessment.

In this step there is no cut-off criteria so the LCA is conducted for all impacts categories and the final assessment will reflect the level achieved as well as the detailed score in each impacts category as illustrated in Table 8. Note that the application of this evaluation system will be tested with the case-studies.

Figure 17. Workflow relevant to Step 4 of the SSbD framework. Please note that this scheme refers to steps to be followed to assess environmental sustainability and is not entailing exclusion criteria

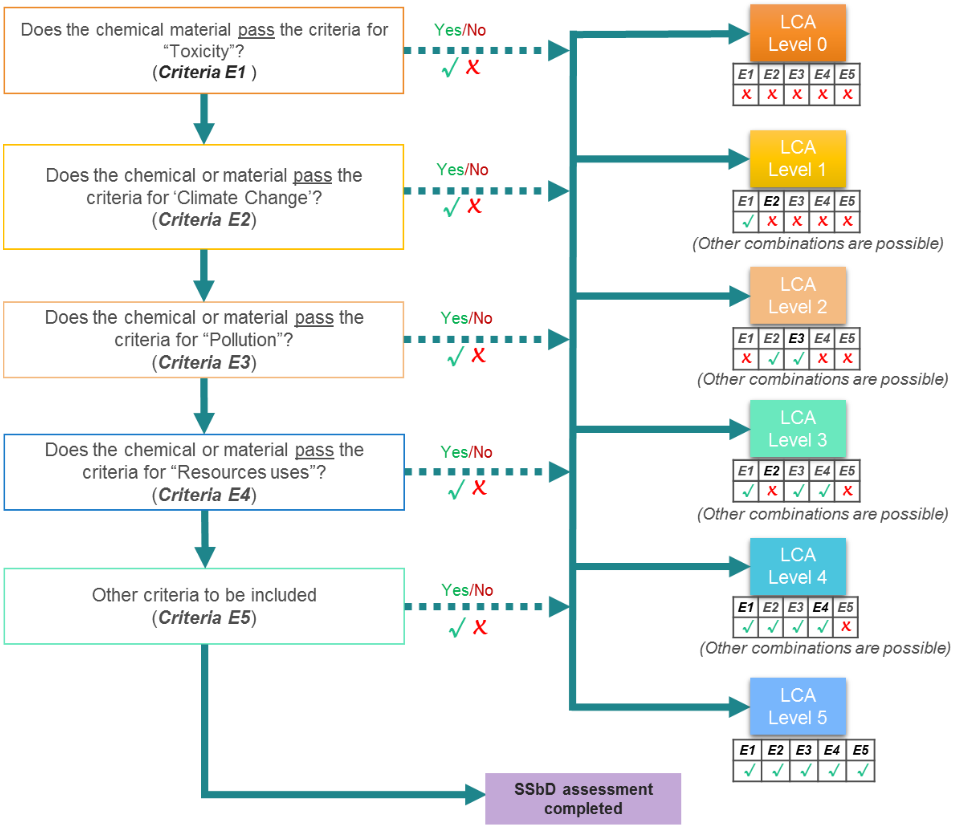

Table 9. Example of a summary table of the evaluation of Step 4

LCA Assessment level (max score)	Aspect	Score	Level
Toxicity ES1 (max 12)	Human Toxicity, cancer	3	✗
	Human Toxicity non cancer	2	
	Ecotoxicity	1	
Climate Change ES2 (max 4)	Climate Change	3	✓
Pollution ES3 (max 32)	Ozone depletion	4	✗
	Particulate matter/Respiratory inorganics	2	
	Ionising radiation, human health	2	
	Photochemical ozone formation	1	
	Acidification	0	
	Eutrophication, terrestrial	4	
	Eutrophication, aquatic freshwater	3	
	Eutrophication, aquatic marine	2	
Resources ES4 (max 16)	Land Use	4	✓
	Water use	2	
	Resource use, minerals and metals	2	
	Resource use, energy carriers	2	

4.2.5 Scientific basis for the socio-economic sustainability assessment (Step 5)

The social and economic dimensions are integral parts of the sustainability concept, but less implemented in the practice of sustainability assessment. In the case of social sustainability, the aim is to protect people's rights in terms of individuals (e.g. as workers, consumers, children, value chain actors) and collectively as communities, while maximizing benefits for society as a whole (UNEP, 2020a). The definition of economic sustainability is more controversial, given that some authors argue that preserving economic growth (which is underpinning the concept of sustainable development) is incompatible with the limits of the planet (Purvis et al., 2019; Ruggerio, 2021).

This section focuses on the scientific basis of the socio-economic sustainability assessment, describing the main available approaches. Given the limited level of its implementation, further work is needed in order to ensure applicability in the framework for SSbD chemicals and materials.

Concerning the scope of Step 5, only social and economic aspects not assessed in previous steps are taken into account. Occupational health and safety is partially addressed in Step 2 of the SSbD framework in terms of hazards and risks from processes related to chemicals and materials. Safety aspects related to accidents at work are instead part of the social assessment.

Two main features characterise the social sustainability assessment:

- The stakeholder perspective, i.e. the need to explicitly take into account various actors and the potential impact affecting them. It implies the identification of relevant stakeholders in the various steps of the life cycle of the chemical or materials and the existence of potential conflicting interests between them.
- Positive impacts are part of the social assessment and can be of three typologies, according to the current state of the art (Di Cesare et al., 2016):

  Type A – Positive social performance going beyond business as usual (e.g. improving workers skills beyond legal requirements);

  Type B – Positive social impact through presence of an economic activity (e.g. creation of employment);

  Type C –. Positive social impacts resulting from the intrinsic characteristics of the product utility (e.g. in the case of products aiming at improving the well-being of people). This type of impact is rarely assessed in S-LCA, as there are different views on whether it is relevant, warranted and fair to account for the positive social impacts related to the product utility (UNEP, 2020).

The assessment of positive impacts is conceptually very important in order to recognise and quantify the contribution that economic activities can provide to the achievement of Sustainable Development Goals and in order to incentivise companies to advance in their sustainability strategies. Some conceptual and methodological challenges, however, have hindered the assessment of positive impacts in the practice (Croes and Vermeulen, 2019). For instance, the aggregation of positive and negative impacts should be avoided in order to prevent compensation; the absence of negative impacts should not be accounted as positive impacts, especially in the context of assessing (or aiming to) absolute sustainability.

Concerning the assessment of economic aspects, this section provides general indications on the potential scope of an economic analysis. In particular, the analysis focuses on non-financial aspects, e.g. the identification and monetization of externalities arising during the life cycle of a chemical or a material. It does not include internal costs management, which are part of the company own business administration.

The assessment of socio-economic considerations can rely on existing Life Cycle based methodologies, namely the Life Cycle Costing (LCC) (Rödger et al., 2018) and the Social Life Cycle Assessment (S-LCA) (UNEP, 2020). These methodologies, however, are less mature than the environmental one. Some methodological challenges have not been solved yet, and their application in case studies is more heterogeneous compared to the environmental LCA. For this reason, only general information on the available approaches is provided in this context.

Social assessment

The UNEP S-LCA Guidelines recommend considering six stakeholder categories in the assessment of social impacts: workers, local communities, consumers, (other) value chain actors, society and children. Forty social aspects (defined in S-LCA as impact subcategories) should be addressed, selecting the most relevant ones for the assessment and providing a justification for their exclusion (UNEP, 2020).

The Product Social Impact Assessment Handbook, a guidance developed by companies involved in the Roundtable for Product Social Metrics (Goedkoop et al., 2020), proposes four stakeholder categories (workers, users, local communities and small-scale entrepreneurs) and 25 social topics.

The Social Life Cycle Metrics for Chemical Products was developed by the World Business Council for Sustainable Development (WBCSD, 2016). It is an initiative of the chemical industry aiming at providing methodological guidance on measuring and reporting social impacts of chemical products along their life cycle. It includes three stakeholder categories (workers, local communities and consumers), 11 compulsory social categories and 14 additional categories to be selected by the practitioner.

In literature, the stakeholder categories that are mostly used are workers, local communities and consumers (Desiderio et al., 2021).

Given the objective of this framework, i.e. presenting the dimensions, aspects, and indicators that can be used to assess chemicals and materials and how criteria can be defined in order to identify those that are SSbD, a streamlined and operational set of social aspects could be prioritised from the available frameworks on social assessment.

The selection of aspects was carried out comparing a set of relevant frameworks, listing the social aspects they cover and selecting those that appear most frequently. The following frameworks have been analysed:

- UNEP S-LCA Guidelines 2020 (UNEP, 2020)
- Product Social Impact Assessment Handbook (Goedkoop et al., 2020)
- Social Life Cycle Metrics for Chemical Products was developed by the World Business Council for Sustainable Development (WBCSD, 2016)
- The European Chemical Industry Council, Cefic Safe and Sustainable by Design report (Cefic, 2022)
- The Social Taxonomy developed in the context of the EU Sustainable Finance process (Platform on Sustainable Finance, 2022c)
- The Guidelines for the EU Non-Financial Reporting Directive (EC, 2017)
- The results of the review of safety and sustainability dimensions, aspects, methods, indicators and tools for safe and sustainable by design chemicals (Caldeira et al., 2022).
- OECD Guidelines for Multinational Enterprises, which is the main standard for responsible business conduct (OECD, 2011).

The full list of aspects covered by the frameworks considered in writing this document is presented in the Annex 6 (Table A6.1). A total of 83 social aspects have been identified, belonging to seven stakeholder categories (the six categories proposed by the UNEP Guidelines and the additional category proposed in the Product Social Impact Assessment Handbook, i.e. small-scale entrepreneurs). Five social aspects for the workers category have been included in all the frameworks under investigation: freedom of association and collective bargaining, child labour, fair salary, forced labour, health and safety. As emerged from the review of Desiderio et al. (2022), workers, local communities and consumers are the stakeholder categories with the highest frequency of commonly considered social aspects. The aspects mentioned in at least five frameworks are mentioned in the Table 10.

Table 10. List of stakeholder categories, social aspects and occurrence in the social frameworks under investigation

Stakeholder category	Social aspect	Number of frameworks including the aspect
Workers	Child labour	8
	Fair salary	8
	Forced labour	8
	Health and Safety	8
	Freedom of association and collective bargaining	7
	Working hours	7
	Equal opportunities / discrimination	7
Local community	Community engagement	6
	Local employment	6
Consumers	Health and safety	7
	Responsible communication	6

Indications for further testing

In the case of a company willing to perform a social assessment, the analysis should focus on:

- Assessment of own operations, using primary data that can be provided by the company or collected in local communities.
- Assessment of the supply chain, and scrutiny of suppliers' operations. This should be based, as much as possible, on a specific analysis, thus collecting primary data and information from suppliers. When this information is not available or is not possible to collect specific information, secondary data can be used. For instance, specific S-LCA databases contains information on social risk of country-sectors combinations for a wide range of social aspects. Specifically, these are the Social Hotspot Database and the Product Social Impact Life Cycle Assessment (PSILCA) database. Potential additional data sources for secondary data are listed in the Table A5 in the Annex.

A recently published report provides guidance on how to implement the UNEP S-LCA guidelines in real case studies and can guide in performing the social assessment of a chemical product as explained above (Life Cycle Initiative and Social Life Cycle Alliance, 2022).

Table A6.2 in Annex 6 illustrates the indicators that can be used to evaluate the social aspects selected from the framework, based on the UNEP methodological sheets for Subcategories in Social Life Cycle Assessment (UNEP, 2021). The health and safety aspects, related to both workers and consumers, are also covered in step 2 of the framework and therefore are treated here only for what concerns additional aspects not included in the safety assessment, i.e. the assessment of accidents at work.

Concerning the assessment of social impacts, the outcomes of the EU Horizon 2020 project Orienting[44] (ID: 958231), aiming at identifying the best available approaches for Life Cycle Sustainability Assessment, recommends the reference scale approach (Harmens and Goedkoop, 2021). Indeed, compared to other available methods, the reference scale is the most feasible and operational. This approach is also adopted in the World Business Council for Sustainable Development report (WBCSD, 2016), providing guidance on how to assess and report on the social impact of chemical products. The reference scale approach translates the performance of system/organisations' activity into an evaluation of potential impacts. The method sets, for each indicator, various levels of social performance or social risk. The reference scales then combine the indicator value with performance reference points (PRP) corresponding to different levels of performance compared to thresholds, targets or objectives. Legislation, standards, international conventions and other normative tools can be used

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[44] https://orienting.eu/

as sources to extract these critical levels and define what can be considered a satisfactory or a deficient performance (Caldeira et al. 2022).

Economic assessment

Within the sustainability concept, the economic dimension is linked to achieving economic growth considering the resource-constrained world's environmental and social implications. However, there is no shared definition of economic sustainability and economic indicators can be linked to different costs linked to the production of a product e.g. capital or operating costs but also societal or environmental costs. (Caldeira et al. 2022).

In life cycle sustainability assessment, the economic pillar is usually addressed through the Life Cycle Costing (LCC) methodology. Prior to its use in sustainability assessment, LCC was also used in pure economic analysis and intended as a concept aiming at "optimizing the total costs of asset ownership, by identifying and quantifying all the significant net expenditures arising during the ownership of an asset" (Woodward, 1997). Nowadays, various forms of LCC have been developed and applied in literature, even though their level of methodological maturity is still low, particularly for the forms of LCC combining societal impacts. Before introducing the main forms of LCC, the following definitions are provided:

- internal costs are borne by actors directly involved in the life cycle of the product;
- external costs (also termed externalities) are value changes caused by a business transaction, which are not included in its price, or value changes caused as side effects of the economic activity (Rödger et al., 2018).

Based on the definitions above, three types of LCC can be described (Bianchi et al., 2021):

- The conventional LCC (cLCC), which focuses on internal costs and is a pure economic evaluation taking into consideration the different stages in a life cycle approach.
- The environmental LCC (eLCC), which extends the LCC by including environmental externalities and a comprehensive multistakeholder perspective. This methodology built upon the same product system as an environmental LCA and compared to the cLCC it broadens the perspective by looking at one or several actors along the whole life cycle of a product.
- The societal LCC (sLCC), which further extends eLCC by including additional externalities, associated with the life cycle of a product. Therefore, sLCC assesses all costs associated with the life cycle of a product that are covered by anyone in society, whether today or in the long-term future. The perspective of sLCC comprises the society overall (locally, as well as nationally and internationally), also including governments. This is the least developed methodology within the LCCs, being applied only in a case study in the literature (Bianchi et al., 2021).

The list above is not exhaustive, as several other approaches have been suggested in literature. For instance, LCC is also increasingly applied to evaluate the economic consequences of improving circularity in product systems. While this approach is not yet formalised in a standardised methodology, using cicular economy related approaches in LCC has the benefit of taking into account the value generated by re-circulating or extending the useful life of the products components/materials. This kind of evaluations allows calculating a so-called cost-footprint, i.e. assessing the total costs incurred for a product by all stakeholders involved during the entire time period and all life cycles of use (Bradley et al., 2018; Wouterszoon Jansen et al., 2020).

Other economic considerations can concern the use of Critical Raw Materials (Blengini et al., 2017), i.e. materials having high economic importance and high supply risk. Even though this type of assessment is usually not included in the traditional sustainability assessment, the use of materials having high geopolitical concern could be easily implemented also within the environmental LCA, given that the presence of critical materials can be easily tracked in the Life Cycle inventory phase (Mancini et al., 2015).

Indications for further testing

This section provides general indications on the methodology that could be used to assess the economic sustainability of chemicals and materials, acknowledging the limited development of the available approaches.

Given the scope of this framework, the eLCC could be used as a methodology for the economic sustainability assessment of chemicals and materials. Indeed, as stated in section 3.3, the ambition of the economic assessment in the context of the framework herein presented is on the identification and evaluation of externalities, rather than on the assessment of internal costs, that is part of the usual business administration. While the sLCC is conceptually interesting for the purposes of this framework, it is not developed enough from a methodological point of view to be operational. Applying the eLCC methodology could be convenient from the operational point of view, as it can be built on the same model used in step 4 for the environmental analysis (LCA), and requires the identification of stakeholders, which is needed also in the social assessment.

A crucial part of the economic assessment lies in the quantification of externalities through monetization. Monetary valuation is the practice of converting measures of social and biophysical impacts into monetary units and is used to determine the economic value of non-market goods, i.e., goods for which no market exists (Pizzol et al., 2015). Various approaches and methods can be used to perform monetary valuation. For instance, using market prices (observed preferences), market prices of a surrogate (revealed preferences), determining willingness to pay in hypothetical markets or trade-off situations (stated preferences), determining potential cost for the marginal abatement or replacement activity (abatement cost), etc.

Monetary evaluation can also be used to compare different impact categories results in a LCA study. The availability of factors converting environmental impacts in monetary values (Monetary Value Coefficients, MVCs) varies significantly across impact categories. Some impact categories are commonly analysed in literature with several MVCs available from different sources (e.g., climate change and ozone depletion), whilst other impact categories are not extensively studied and few MVCs are available to date (e.g., eutrophication, terrestrial and land use) (Amadei et al., 2021). A monetary valuation of environmental impact results deriving from the LCA study could be performed in order to integrate the assessment with economic considerations. The results of the economic assessment related to externalities could be an additional part of the framework and not necessarily be integrated in the scoring system used in the other steps.

5. Evaluation procedure

As presented in the previous sections, the assessment of an SSbD chemical/material entails many aspects that need to be evaluated individually and, to support decision making, combined.

Aggregation of aspects may facilitate decision, but in the context of SSbD it is important to note that the use of aggregation methods does not rule out a richer dashboard presenting not only the overall aggregate result, but also the results obtained in other levels of the hierarchy. Such information is important to understand the strengths and weaknesses that an aggregate result inevitably might hide and therefore we consider the presentation of the detailed information of the assessment essential, and a key component of the evaluation as described in section 5.1.

For the aggregation of the different aspects, we propose the use of Multi-criteria Decision Aiding (or Analysis) (MCDA), a field of Operational Research, Management Science and Decision Theory devoted to the study of decision-making when multiple evaluation dimensions are involved (see, e.g., Belton and Stewart, 2002; Greco et al., 2016; Ishizaka and Nemery, 2013). MCDA has been highlighted as a key instrument for sustainability assessment, as discussed in major works and reviews by Munda (2005), Cinelli et al. (2014), Ibánez-Forés et al. (2014), Diaz-Balteiro et al. (2017), or Lindfors (2021). Considering the most relevant characteristics of the SSbD evaluation framework, MCDA methods that can potentially be applied for the aggregation of the different aspects are presented (section 5.2). These options will be tested during the case studies development.

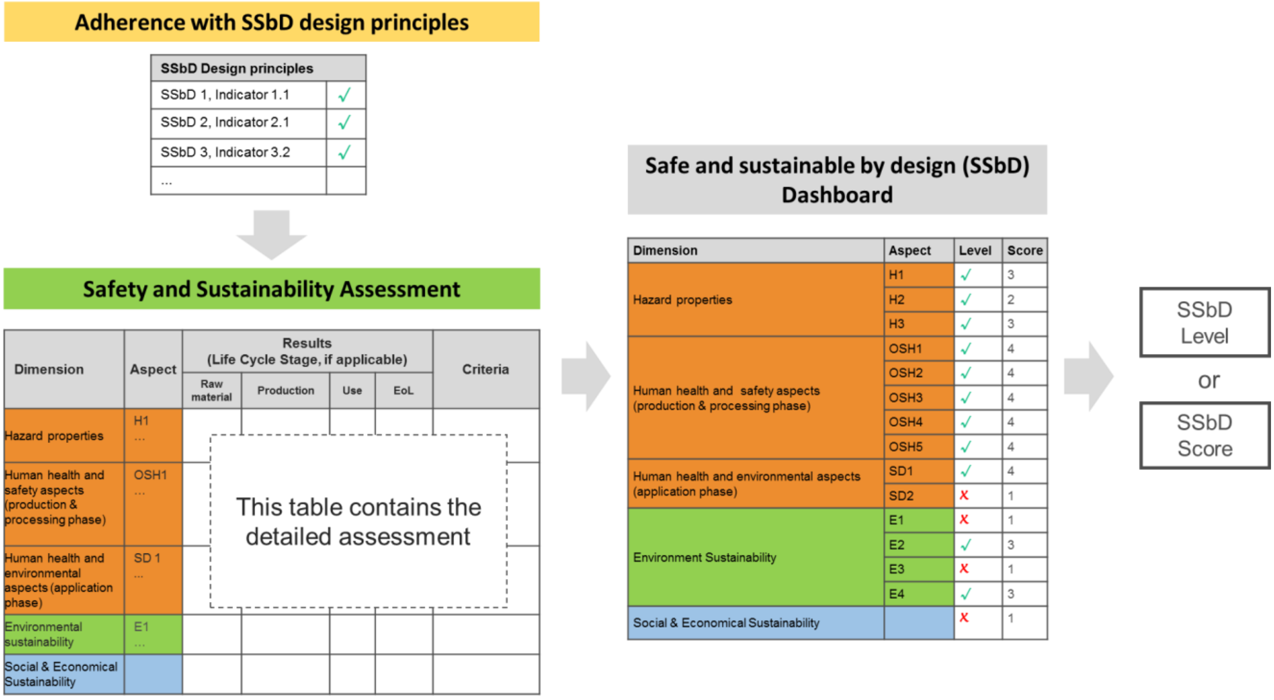
5.1 Adherence with SSbD principles and safety and sustainability assessment

As illustrated in Figure 18, the application of the framework will provide three outputs:

1. The adherence to the SSbD principles during the design phase;
2. The safety and sustainability assessment, namely the detailed figures on the performance of the chemical/material against the SSbD criteria;
3. A dashboard summarising the results of the safety and sustainability assessment is proposed as a tool to facilitate informed conclusions/decisions based on a holistic assessment.

The reporting of adherence to SSbD principles is optional, whilst the most important and essential component is the detailed assessment of the performance of the chemical/material in the different aspects assessed to ensure transparency in applying the framework and the identification of hotspots.

Figure 18. Illustration of the evaluation components. Socio-economic aspects are only represented for completeness as these are still being in an exploratory phase



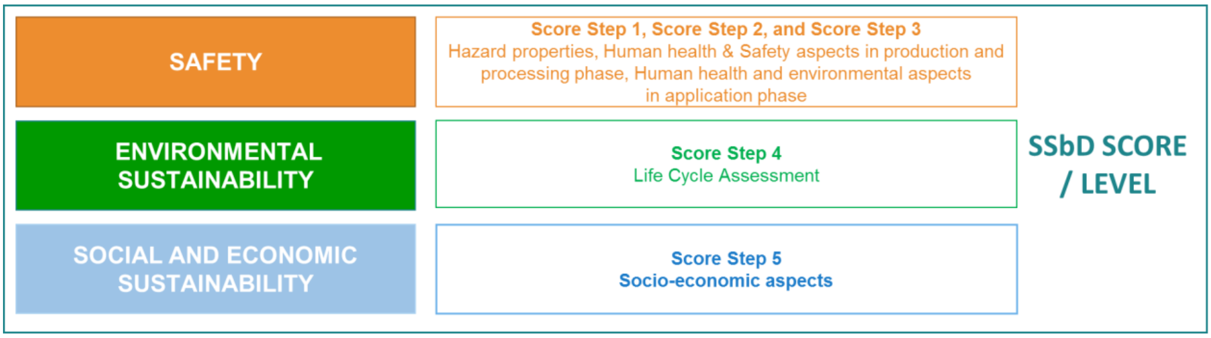
SSbD Design principles	
SSbD 1, Indicator 1.1	✓
SSbD 2, Indicator 2.1	✓
SSbD 3, Indicator 3.2	✓
…	

Dimension	Aspect	Results (Life Cycle Stage, if applicable)				Criteria
		Raw material	Production	Use	EoL	
Hazard properties	H1 …					
Human health and safety aspects (production & processing phase)	OSH1 …					
Human health and environmental aspects (application phase)	SD 1 …					
Environmental sustainability	E1 …					
Social & Economical Sustainability						

Dimension	Aspect	Level	Score
Hazard properties	H1	✓	3
	H2	✓	2
	H3	✓	3
Human health and safety aspects (production & processing phase)	OSH1	✓	4
	OSH2	✓	4
	OSH3	✓	4
	OSH4	✓	4
	OSH5	✓	4
Human health and environmental aspects (application phase)	SD1	✓	4
	SD2	✗	1
Environment Sustainability	E1	✗	1
	E2	✓	3
	E3	✗	1
	E4	✓	3
Social & Economical Sustainability		✗	1

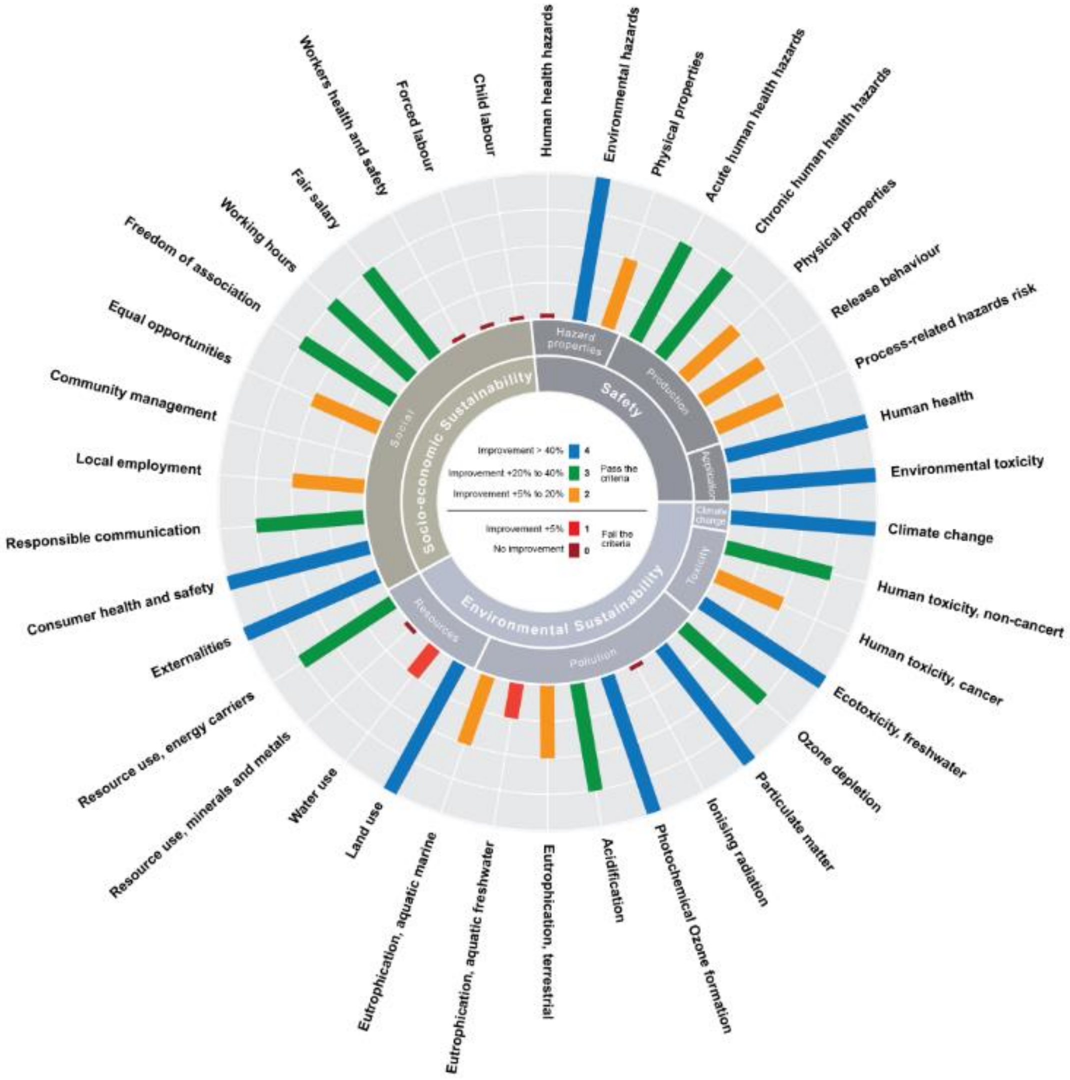
The final result of the evaluation can be expressed either as a class of SSbD (poor, good, very good) or with a numerical score derived from the combination of the individual scores in each aspect (subject to e.g. weighting). These options will be explored with the case studies considering the options presented in section 5.2.

Figure 19. Overall evaluation procedure combining the assessment results of all dimensions



As mentioned before, one of the options envisaged for the evaluation is to have a score per each step described in sections 4.2.1 to 4.2.5 and the aggregation of the different scores would result in a SSbD SCORE (as illustrated in Figures 18 and 19). As introduced in section 3.3, the evaluation procedure is underpinned by a hierarchical principle in which a first step is to assess specific safety aspects that are mandatory and with exclusion criteria. Only those chemicals/materials that pass this first step are then considered and evaluated for their 'SSbD SCORE'. This score has three components, a component that reflects the safety assessment, another which shows the result of the environmental sustainability assessment, and in the future possibly a third one that includes other aspects of the social and economic sustainability assessment. An illustrative example for visualisation of the evaluation results for each aspect considered is presented in Figure 20. The chemical/material should be considered SSbD if passing the criteria defined for safety and environmental sustainability described in the previous section. The idea of a scoring system is to allow to rank those that are SSbD and those that are not. Those that are not considered as SSbD can be flagged for improvement (e.g. redesign of the production process taking into account principles for SSbD presented in section 4.1) or for substitution.

Figure 20. Overview of dimensions and aspects considered in the framework and illustrative example for visualisation of the evaluation results. Socio-economic aspects are represented for completeness as these are still being in an exploratory phase



5.2 Multiple-criteria decision analysis (MCDA) to support decision making in SSbD

The SSbD framework proposed defines a set of requisites to be taken into account when suggesting an overall evaluation procedure. Table 11 lists the main requisites and their implications.

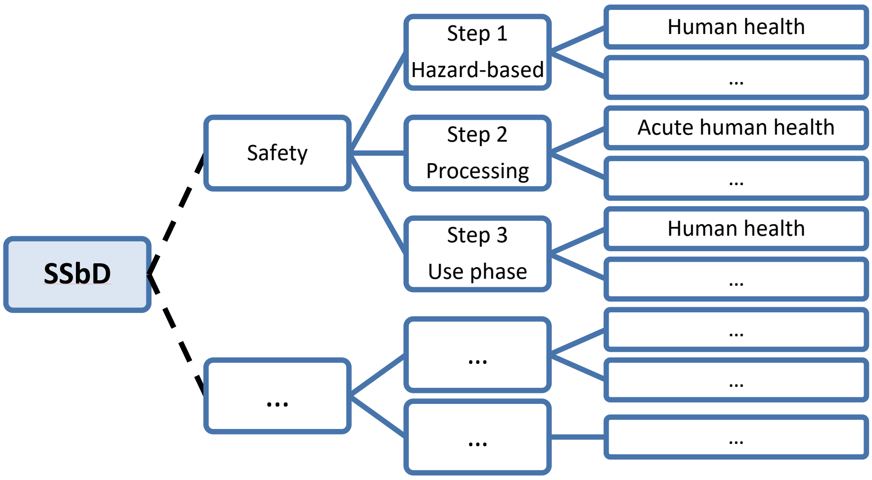
Table 11. SSbD framework requisites and their implications regarding the application of MCDA

SSbD framework requisites	Implications
1. The evaluation procedure can be applied to new chemicals and materials or to existing ones	By including new chemicals and materials, data quality can vary widely among aspects (or attributes, the term used in MCDA)
2. The evaluation procedure shall take into account the lack of data and data uncertainty	Data quality needs to be assessed
3. The result of the evaluation can be expressed either as a class of SSbD (poor, good, very good) or with a numerical score derived from the combination of the individual scores in each aspect	The result can be provided on an ordinal scale as a qualitative level, i.e. a rating (Colorni and Tsoukiàs, 2021). Alternatively, it can be a continuously varying numerical value.
4. A criterion is defined as an aspect with an assessment method and a minimum or maximum threshold or target values, on which a decision may be based	Each attribute is associated with thresholds to act as classification criteria. A qualitative level (rating) is obtained for each attribute. The numerical values to be compared with the thresholds might be also available.
5. The ambition of the SSbD is to move from relative (safer and more sustainable) to absolute (safe and sustainable) improvements ensuring that chemicals and materials are produced and used without exceeding acceptable boundaries.	The procedure should evaluate each chemical or material based on its own merits (absolute evaluation independent from other chemicals or materials being assessed).
6. The chemical/material should be considered SSbD if passing the criteria defined for safety and environmental sustainability	No trade-offs allowed between safety and environmental performance. One dimension cannot compensate for weaknesses on the other dimension.
7. The evaluation procedure is underpinned by a hierarchical principle. A 'step score' and an 'overall SSbD score' could be developed considering the combination of scores. If the minimum criteria for safety dimension are not met, then the chemical/material cannot be considered as SSbD.	The aggregation approach should respect the predefined hierarchy. A poor safety assessment cannot be overridden by the environmental assessment.

5.2.1 Possibilities for multiattribute aggregation

The application of the criteria presented in the previous sections results in multiple assessments that can be combined using MCDA. Multiattribute aggregation methods can be used both to aggregate multiple aspects encompassed in a single dimension at different levels of an aggregation hierarchy (Figure 21) and to aggregate the top-level dimensions (safety, environmental sustainability, etc.).

Figure 21. Hierarchy of assessment attributes



The considerations in this section are based mainly on the requisites and implications identified in Table 12, and derive from the following three essential characteristics of the aggregation process:

a) Absolute vs. relative assessment

Based on the required characteristics, relative multiattribute aggregation methods (those for which the evaluation of one alternative depends on other alternatives being assessed at the same time) should be excluded for three reasons: first, an absolute rather than a relative assessment is sought (Requisite 5 in Table 12); second, it should be possible for an organisation developing a new chemical or material to assess if it is SSbD, without needing to obtain data on all of its possible competitors; and third, because rank-reversals (e.g. A is better than B if C is not considered, but B is better than A if C is present) (Wang and Luo, 2009) are better avoided.

b) Input and output scales

For the third requisite in Table 12, the result should be a rating class (e.g. “Green”, “Yellow”, “Red”) or a cardinal value in an interval scale (e.g. 56.78). Using numerical levels (e.g. the number of stars in a hotel) does not necessarily correspond to cardinal values if these numerals could be replaced by non-numerical levels. To be considered an interval scale, equal differences between levels must correspond to the same meaning concerning what is being measured (e.g. the difference between a “1” and a “2” is as important or as valued as the difference between a “2” and a “3”). Interval scales can be converted into ratings by eliciting thresholds separating the consecutive levels. In the reverse direction, conversion of ratings into interval scales requires eliciting a value function, through a direct or an indirect elicitation protocol (Morton and Fasolo, 2009; Morton, 2018).

The option of using rating scales for the SSbD framework presents several advantages:

- It is well aligned with many existing scoring or certification schemes proposed by different entities (Caldeira et al, 2022, p. 85);
- It lends itself to an easy interpretation;
- It suits well the association between levels and actions, e.g. level 3 might entail “Pass”, etc.;
- It fits assessments based on qualitative properties (e.g. carcinogenic category, being flammable, etc.) rather than numbers;
- It avoids an illusory perception of precision when reading results;

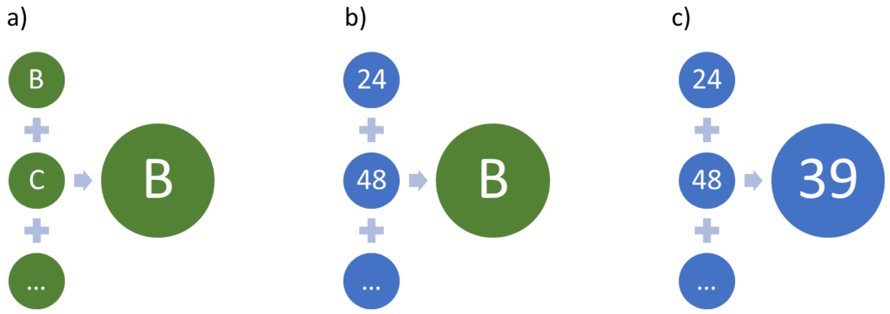
- It allows a greater stability of the assessment result with regards to some uncertainties.

On the other hand, using an interval scale for the SSbD framework also has some advantages:

- It preserves the maximum amount of information in the aggregation step (e.g. it is a B, but very close to an A);
- It allows more discrimination when comparing alternatives;
- It is not difficult to translate results as a rating subsequently.

If the inputs scale for the attributes is an interval scale, it is possible to convert it at any moment to a rating scale, but the contrary is considered to be harder. The possible pathways along the aggregation hierarchy can are illustrated in Figure 22.

Figure 22. Aggregation: a) rating to rating; b) cardinal to rating; c) cardinal to cardinal



c) Compensation among attributes

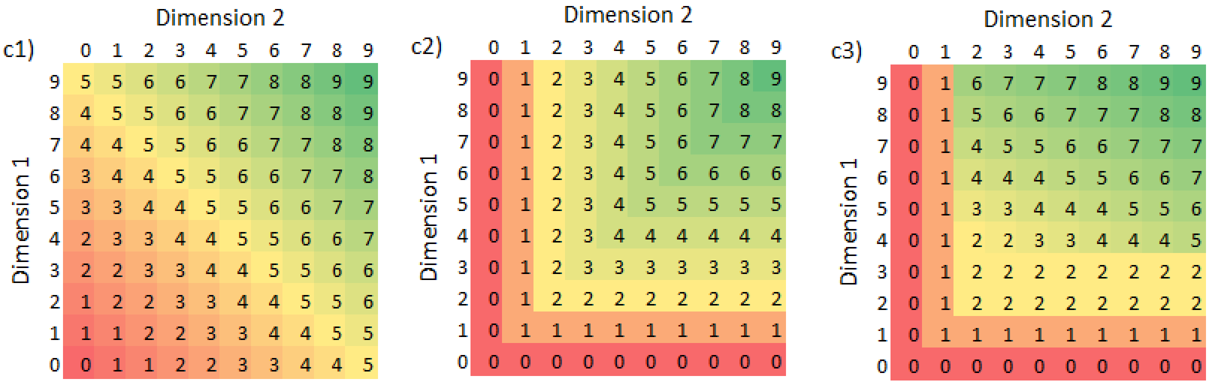
Compensation means the possibility that very poor performance on one attribute might be compensated by very good performance on some other attributes. The compensatory vs. non-compensatory dichotomy in aggregation methods (limited on some methods but fully allowed in other methods) has been related with the issue of weak vs. strong sustainability (Munda, 2005). Figure 23 illustrates different types of compensation for a case of aggregating two attributes:

- In case c1) an additive aggregation is used weighting equally the two dimensions. Improving one unit in one dimension compensates exactly worsening one unit in another dimension.
- In case c2) the aggregation corresponds to the minimum. No compensation occurs.
- In case c3) some compensation exists but it is limited in te sense that very poor performances cannot be compensated.

Aggregation can be used for the different steps proposed in this framework. For instance, in the Safety dimension, one can aggregate the assessment of the first three steps, concerning the hazards assessment, the production and processing risk assessment and the use phase risk assessments. In turn, each of these attributes entail the aggregation of other attributes.

For some of the steps, the input scales already define a specific type of aggregation. This is the case of Step 1 (intrinsic hazard), for which a set of rules based on passing three criteria (conditions) defines whether the chemical is rated Level 0, Level 1, Level 2 or Level 3. This rating is then an input for the aggregation of Safety at the next level of the hierarchy (Figure 21). At that stage, then, a method to aggregate ratings should be used (type a) in Figure 22). For other steps, more freedom exists to choose an aggregation method. For instance, under the Environmental sustainability dimension the inputs are initially cardinal (% above or below target level), and then translated into 5 rating levels. Therefore, both aggregations based on the ratings or aggregation based on the initial interval scales can be considered.

Figure 23. Aggregation of 0-9 interval scales at the top level. (c1) average; c2) minimum; c3) mix of weighted sum and minimum emphasising Dimension 1)



c1)

Dimension 2

Dimension 1	0	1	2	3	4	5	6	7	8	9
9	5	5	6	6	7	7	8	8	9	9
8	4	5	5	6	6	7	7	8	8	9
7	4	4	5	5	6	6	7	7	8	8
6	3	4	4	5	5	6	6	7	7	8
5	3	3	4	4	5	5	6	6	7	7
4	2	3	3	4	4	5	5	6	6	7
3	2	2	3	3	4	4	5	5	6	6
2	1	2	2	3	3	4	4	5	5	6
1	1	1	2	2	3	3	4	4	5	5
0	0	1	1	2	2	3	3	4	4	5

c2)

Dimension 2

Dimension 1	0	1	2	3	4	5	6	7	8	9
9	0	1	2	3	4	5	6	7	8	9
8	0	1	2	3	4	5	6	7	8	8
7	0	1	2	3	4	5	6	7	7	7
6	0	1	2	3	4	5	6	6	6	6
5	0	1	2	3	4	5	5	5	5	5
4	0	1	2	3	4	4	4	4	4	4
3	0	1	2	3	3	3	3	3	3	3
2	0	1	2	2	2	2	2	2	2	2
1	0	1	1	1	1	1	1	1	1	1
0	0	0	0	0	0	0	0	0	0	0

c3)

Dimension 2

Dimension 1	0	1	2	3	4	5	6	7	8	9
9	0	1	6	7	7	7	8	8	9	9
8	0	1	5	6	6	7	7	7	8	8
7	0	1	4	5	5	6	6	7	7	7
6	0	1	4	4	4	5	5	6	6	7
5	0	1	3	3	4	4	4	5	5	6
4	0	1	2	2	3	3	4	4	4	5
3	0	1	2	2	2	2	2	2	2	2
2	0	1	2	2	2	2	2	2	2	2
1	0	1	1	1	1	1	1	1	1	1
0	0	0	0	0	0	0	0	0	0	0

The aggregation possibilities for each type of scale are discussed next (see Figure 22):

a) Aggregation of rating levels given as an input to provide an output as a rating level

Aggregation based on IF-THEN rules is a possible way to aggregate rating levels, although if the number of attributes is high then the number of rules to be defined can be high as well. Rule-based MCDA methods to deal with a large number of rules include Decision EXpert (DEX) (Bohanec et al. 2013) and Dominance based Rough Set Approach (DRSA) (Greco et al., 2016). A second possibility is to use a qualitative version of the ELECTRE TRI method (Dias et al., 2018). This method implements a concordance-discordance voting analogy, in which a rating level is granted if it is supported by a sufficient majority of the attributes without strong opposition from any attribute.

b) Aggregation of interval scales given as an input to provide an output as a rating level

The methods proposed above in a) can be used in this situation after converting cardinal values to a rating scale, but this conversion is however not necessary and would lead to some loss of information. Methods such as the ELECTRE TRI method (Figueira et al., 2013; Yu, 1992) or FlowSort (Nemery and Lamboray, 2008) can be used instead. These are rating methods aggregating multiple interval scales onto a qualitative rating.

c) Aggregation of interval scales given as an input to provide an output on an interval scale

This is the case where more MCDA aggregation methods are applicable, but methods such as a simple average or a weighted sum (Figure 23 c1)) are not recommended when entailing the possibility that a very poor performance on some criterion can be easily compensated, contradicting the spirit of the framework. On the opposite extreme, taking the minimum performance (Figure 23 c2)) does not encourage improvements in one attribute above the minimum in the other attributes. Methods that allow some compensation but within a limited scope might be preferable, including for instance the multilinear form of a multiattribute utility function (Keeney and Raiffa, 1993), the Ordered Weighted Average (Yager, 1988), or methods based on measuring the distance to some ambitious reference (not attained by any of the chemicals to be assessed).

Strategy a), consisting in an aggregation of rating levels given as an input to provide an output as a rating level, offers the advantages of expressing the result as a qualitative rating, with the additional advantage of keeping the same logic used in Step 1 and Step 3 of the safety assessment. Following a concordance-discordance logic is easy to communicate, and its parametrisation allows establishing veto conditions for granting the highest ratings.

Strategy b), consisting in an aggregation of interval scales given as an input to provide an output as a rating level, also has the advantages of expressing the result as a qualitative rating. Among the possibilities considered (DEX, DRSA, ELECTRE TRI, FlowSort), the choice of ELECTRE TRI stands out as being perfectly aligned with the proposal for strategy a), which leads to a more harmonious evaluation framework if strategy a) is used in other nodes of the hierarchy. The possibility of using DEX or DRSA can be considered if a decision maker provides classification examples, but the number of resulting IF-THEN rules might hinder an easy interpretation.

Strategy c), in turn, has the advantage of preserving information assessed on interval scales, but cannot be used in nodes of the hierarchy where the inputs are rating levels, at the expense of the overall harmony of the framework. Options within strategy c) for the aggregation of interval scales require the inputs to be assessed on a common scale. Whenever this is not the case and one does not wish to perform potentially arbitrary scale transformations, it might be preferable to use strategy a) or strategy b). Otherwise, the choice of the evaluation method will depend on the preferences towards their properties and the towards the output scale, possibly considering the overall harmony of the framework.

These options will be further discussed and tested in the case studies in order to select the most appropriate solution for the SSbD evaluation.

6. Data availability and uncertainty

Generally, the SSbD approach and the assessment should be a transparent process, e.g. all necessary information for classification and checking the criteria should be available, including any data gaps and data quality criteria, regardless of the assessment results at the innovation/development stage, ensuring a full tracking of the assessment performed along the life cycle of the chemical or material. Moreover, the broad scope of framework requires extensive amount of data at manufacturing level and supply-chain level.

To achieve these goals, data should be made available among the industry stakeholders, which requires systemic changes in the chemical industry. Emerging tools in the field of artificial intelligence (AI) and digitalization can play a relevant role in supporting this change and fostering research and innovation.

Digitalisation can be an enabler for the innovation in several ways, such as:

- Easier identification of the customer-defined function,
- Creation of digital twins (i.e. digital model of a physical system as a manufacturing plant) for simulation and optimisation of industrial processes,
- Development of advanced control strategies using real-time monitoring and artificial intelligence,
- Prediction of market needs in order to avoid over-production,
- Prediction of physicochemical properties during the design of a chemical.

The digitalization of the complete system of chemical processes can be the solution to particularly complex challenges related to data such as the estimation of environmental aspects of sustainability, such as toxicity and degradability or the mapping detailed chemical flows for complex multi-material products (Fantke et al. 2021). However, factors such as the complexity of the chemicals (i.e. composition definition and variability) and of the supply chains, confidentiality and intellectual property play against the digitalisation of the sector because this paradigm shift requires that data are collected in accessible platforms to share among stakeholders and needs to be categorised and labelled to be machine-readable.

In this context, examples of the use of Artificial Intelligence (AI) includes application of AI to chemical and sustainable processes to improve the process energy efficiency, environmental burdens and operational risks of chemical production (Liao et al. (2022). AI can be also used as tool to support the decision making related in the fundamental research and practical production of chemicals. In addition, at process level, Mowbray et al. (2022) explains the fundamentals of Machine Learning (ML) and data science, and how they can be linked to process and industrial engineering.

Overall, the digitalisation and improved data collection and sharing is a necessary step, together with assessment metrics and decision-making approaches, to develop ‘chemical data intelligence’ for sustainable chemistry (Weber et al. (2021)).

For what concerns the data on social aspects, data gaps and poor data quality can derive from a low level of data granularity (e.g. data on certain social aspects are available only at country level and are not sector specific), impossibility to measure some aspects (e.g. forced labour, which are illegal phenomena and for which only estimates are available); sensitiveness of certain topics which prevent company from disclosure.

However, some synergies can be expected with the proposal for a corporate sustainability due diligence Directive. Indeed, companies (excluding small and medium enterprises) would be required to identify and, where necessary, prevent, end or mitigate adverse impacts of their activities on human rights, such as child labour and exploitation of workers (EU, 2022). The disclosure of this kind of information could facilitate the assessment of suppliers as described in Step 5.

6.1 Overview of data sources to support the SSbD assessment

Several tools and data sources were collected in the context of previous reports (see Chapter 5.2 in (EC, 2021e) and Section 4.4 in (Caldeira et al., 2022)) and that could be exploited in the context of the SSbD framework testing and demonstration. In any case, in order to perform the assessments described in the framework, each step will require reliable data sources and tools that can process the information.

Thus, the assessment steps refer already to some specific tools that can be used for the case studies demonstration. As a starting point and in addition to the tools already mentioned in the description of the Steps 1-3, sources such as ECHA's Information on Chemicals[45], EFSA' Chemical Hazards Database (OpenFoodTox)[46], OECD's eChemPortal[47], EPA's CompTox[48], etc. that can be screened first, especially for information on hazard properties of existing chemicals. In addition, the topic of data generated using alternatives methods to animal testing is included, as relevant for the safety assessment steps. During the framework demonstration additional data sources should be investigated in order to fill any data gap.

Data availability can also be a challenge for conducting the LCA in as proposed in Step 4 as for the compilation of the inventory, several information on each life cycle stage is required, including primary data collected internally to the organisation performing the assessment or supply-chain specific data for the chemical/material under assessment. For raw material extraction and acquisition stage, secondary data on chemicals, materials and energy can be used (i.e. data that are not specific of the organisation performing the assessment). The common practise in LCA is to look for secondary data in commercial or open-source database, which collect LCI for different processes. Nonetheless, the current databases do not cover all the possible chemicals and materials, therefore more development is required on this topic to cover data gaps, for example with a procedure for selection of proxy data.

An example of available databases for Environmental Footprint LCI datasets is available on the European Platform for Life Cycle Assessment (EC, 2022d), which is created and managed by the EC. A large platform for searching availability of data across different database is the Global LCA Data Access network (GLAD, 2022), which also provides tools for harmonisation of dataset from different sources.

For modelling of the end-of-life scenario, the diversity of data needed as a function of the specific chemical or material assessed makes difficult to pinpoint specific sources of data. A recommended source for general end-of-life statistics, is the EUROSTAT database (EUROSTAT, 2022), which provides data related to waste management in Europe. Additional useful information is published by trade associations of producers which often release studies and statistics on the sustainability of their own sector.

6.2 New Approach Methodologies (NAMs) in the context of SSbD framework

The concept of new approach methodologies (NAMs) is used as an umbrella for various approaches for generating data by using non-animal methods and technologies which may also allow multiple investigations from a high number of samples at the same time (ECHA, 2017b). NAMs refer to the use of individual non-animal methods, such as *in vitro* methods, as well as *in chemico* or *in silico* methods (e.g. QSARs), along with information on exposure. NAMs can be used alone or more typically in combined approaches, such as integrated testing strategies (ITS) or integrated approaches to testing and assessment (IATA). Underpinning the use of NAMs, adverse outcome pathways (AOPs) are a useful concept making use of biological mechanistic pathways relating human and environmental hazard outcomes to early biological events (Nymark et al., 2020; Doak et al., 2022). In the context of REACH (EU, 2006), non-animal approaches relate to the use of *in vitro* and *in silico* methods, grouping and read-across. REACH specifies the standard information requirements (SIRs) in annexes VII to X, providing explicit options for adaptation of the SIRs. In addition, annex XI provides generic provisions

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[45] ECHA Information on Chemicals https://echa.europa.eu/information-on-chemicals

[46] EFSA Chemical Hazards Database (OpenFoodTox) https://www.efsa.europa.eu/en/microstrategy/openfoodtox

[47] OECD eChemPortal https://www.echemportal.org/echemportal/

[48] US EPA CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard/

for using NAMs, beyond those already included in the Test Methods Regulation (EC, 2008), provided they are duly justified and scientifically sound. These generic options include the use of suitable QSAR models and *in vitro* test methods, grouping of substances and read-across, as well as exposure-based adaptations (ECHA. 2016; ECHA, 2017b). The promotion of alternative methods to animal testing (within the 3Rs principle of Replacement, Reduction and Refinement of animal testing (EU, 2010)) is also part of the EU Chemicals Strategy for Sustainability (EC, 2020a) as "*safety testing and chemical risk assessment need to innovate in order to reduce dependency on animal testing but also to improve the quality, efficiency and speed of chemical hazard and risk assessments*". One of the actions under the CSS is to extend the REACH information requirements, including more extensive use of SIRs based on NAMs.

EU policies and legislation call for innovative and more efficient ways of safety testing and chemical risk assessment that do not depend on animal testing. Advanced technologies such as computational models, *in vitro* methods and organ-on-chip devices are being developed, evaluated and integrated to translate mechanistic understanding of toxicity into safety testing strategies. The ultimate goal is to achieve better protection of human health and the environment while supporting EU innovation and industrial competitiveness, without the use of animals. The development and use of non-animal models and methods are also essential for advancing basic, applied and translational research (EC JRC, 2021).

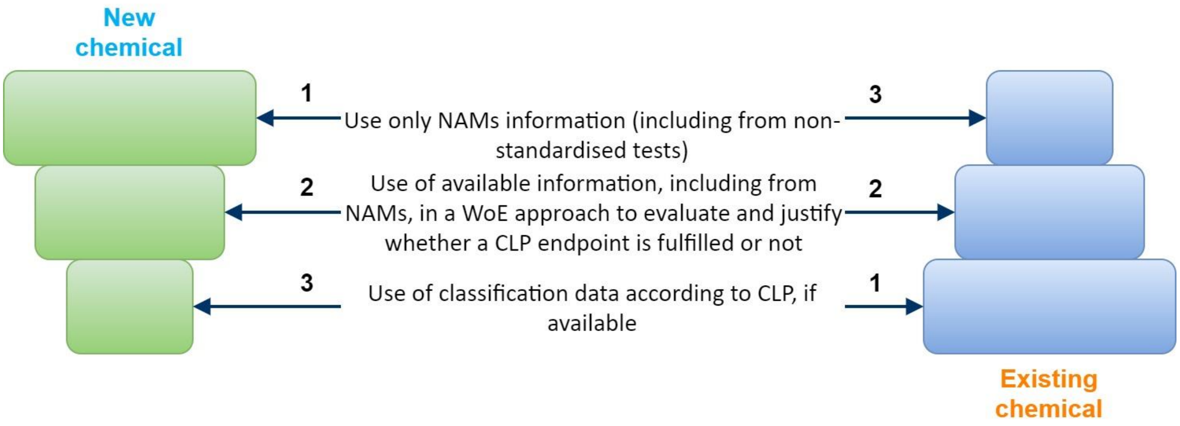
Opportunities for increasing the use of NAMs in legal frameworks, such as CLP and REACH are being discussed in depth. In addition, the SSbD framework should be seen as a tool to support and promote NAMs use, and at the same time, SSbD concept should be a beneficiary of the developments in this area.

In the context of SSbD framework, data generated using NAMs promise to be of utmost importance when hazard properties are investigated. Thus, the role of NAMs and the availability of data becomes central. A non-animal test battery that allows rapid screening for possible hazard concerns in the early phase of the R&D phase as well as comparisons between chemicals would be invaluable in accelerating the transition to SSbD chemicals.

A few considerations regarding NAMs and SSbD:

- Any substance that is considered SSbD should have sufficient hazard data to be completely classified, i.e. sufficient data to apply the classification criteria, thereby ensuring that no hazards are identified at a later point in time (except if new classification endpoints would be defined). This means that for all relevant endpoints sufficient information for classification should be available (including using NAMs, where possible).
- NAMs, are important to guide the process of developing new substances as they are likely to be helpful at early stages in the substance development process (when it is only designed but not yet synthesised).
- Until NAMs will be broadly accepted for regulatory purposes, a tiered approach regarding the information requirements can be adopted (*see Figure 24*) and applied depending on whether a new or an existing chemical is evaluated, to allow the assessment to be performed already at an early stage of the innovation process:
    - Use of classification data according to CLP, if available;
    - Use of available information, including from NAMs, in a Weight of Evidence (WoE) approach to evaluate and justify whether a CLP endpoint is fulfilled or not. For this, information from studies which is conclusive but not sufficient for classification would be used and complemented with NAMs information;
    - Use only NAMs information (including from non-standardised tests) to evaluate and justify whether a conclusion can be made on a hazard endpoint with a sufficient level of confidence.

Figure 24. Tiered approach regarding the information requirements and use of NAMs data for new or existing chemicals



In general, NAMs provide an opportunity for rapid and reliable toxicological profiling of chemicals and materials, including in the design phase. Further consideration should be given to the use of NAM-derived data within the SSbD framework, including the many cases where NAMs provide mechanistic information which is not directly comparable to endpoints from traditional *in vivo* studies.

6.3 Data quality and uncertainty

Data quality and uncertainty is a concern for the different aspects assessed in this framework that needs to be somehow addressed.

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 SETAC, the US Dept. of Agriculture, the US EPA, or the EU JRC (EC, 2021f) 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 Pedrigree Matrix for the impact assessment phase. Although not explicitly based on the Pedigree Matrix, EU JRC’s ILCD and Environmental Footprint methods also use an ordinal 1-5 scale (1↔Excellent, 2↔Very Good, 3↔Good, 4↔Fair, 5↔Poor) with regards to four data quality attributes (Technological representativeness, Geographical representativeness, Time-related representativeness, and Precision).

Having rated multiple data qualitative indicators on such 1-5 scales, some frameworks propose to aggregate them (which is in fact a multi-criteria aggregation problem on its own, for which most of the considerations proposed in Section 5.2 can be relevant). Unfortunately, the most common solution is to compute some sort of average (Lewandowska et al., 2021). This is problematic for two reasons. First, it interprets the “1” to “5” labels as if these were numbers on a cardinal scale. For instance, this assumes the difference between 1↔Excellent and 2↔Very Good is the same as the difference between 4↔Fair and 5↔Poor. Given the nature of the Pedigree Matrix scale, Weidema and Wesnæs (1996) state that any attempt to aggregate the numbers should be avoided. A second reason is the compensatory nature of this aggregation. Using a simple average, having data quality (2,2,2,2,2) (very good overall) is considered to be as good as (5,1,1,1,2), but this single 5 rating (poor) might render the overall results quite uncertain.

Other frameworks have suggested to translate the Pedigree Matrix into probability distributions, either empirically based on existing databases (Ciroth et al., 2016), or based on elicited expert judgment (Qin et al., 2020). Using appropriate uncertainty analysis simulation software, it is then possible to obtain probability distributions for results of interest. At present no consensus exists as to what would be the best process: Qin et al. (2020)'s survey to 47 LCA practitioners shows lack of consensus concerning the use of the Pedigree Matrix, and Edelen and Ingwersen (2018)'s review found authors claiming there is no sound justification for creating probability distributions from data quality assessments.

Another idea that has been put forward is that of incorporating data quality assessment as a means to limit the maximum rating that can be attributed to a chemical. An example is the GreenScreen® method for safety assessment[49]. This method assesses chemicals to provide a qualitative rating on a four levels scale, from Benchmank-1 to Benchmark-4. In parallel, it defines data quality conditions to reach these levels, meaning that a Benchmark-4 chemical might see its rating lowered to Benchmark-3, or even less, due to not meeting the data quality criteria for a higher benchmark.

Additional approaches might be relevant for deriving e.g. a more quantitative measure of uncertainty around SSbD-relevant input data (e.g. Aurisano and Fantke 2022).

More generally, a US National Academies National Research Council (NRC, 2014) defines different ways to cope with uncertainty:

- Using only known best estimates, excluding (not assessing) chemicals with critical data missing.
- Performing uncertainty downgrades (as occurs in GreenScreen®), i.e. downgrading best-estimate values based on uncertainty, thereby punishing alternatives with poor data quality, which is deemed by the NRC to be counter-productive.
- Performing quantitative uncertainty analyses, based on ranges or probability distributions, which NRC deems might be sufficient for some comparative assessments.
  Remaining neutral about uncertainty and missing data, noting the presence of uncertainty and missing data but not excluding the alternative, which is the option the NRC considers better aligned with the nature of their framework.

Considering the SSbD framework, aiming at guiding innovation at early design stages, one should consider what is the purpose of the evaluation. While innovating, often through a trial-and-error process, many data might be missing or be highly uncertain. As the innovation process progresses, some options are discarded, more investment in data gathering occurs, and uncertainties tend to decrease. In these settings, excluding chemicals for which good data does not exist yet, or punishing such chemicals with a lower rating[50] does not seem sensible for the innovators. Therefore, one possibility they have is to remain neutral about uncertainty and missing data, noting the presence of uncertainty, as advocated by the NRC. The innovation team might refer to the obtained rating as the "Estimated SSbD rating", which can be compared with the sought rating as a driver for further innovation and data collection efforts.

A second possibility is to perform quantitative uncertainty analyses that will indicate the probability distribution for the chemical's rating. This requires estimating the input attributes distributions, either in a rough way (e.g. uniform distribution within a plausible range) or in a more specific way, e.g., using distributions derived from a Pedigree Matrix or from an expert panel. The innovation team might refer to the "Most likely SSbD rating", "Median SSbD rating", "Minimum assured SSbD rating", or even to an "SSbD rating 95% confidence interval" to guide their decisions.

Another option can be the calculation of a **data quality score** based on the use of the pedigree matrix in which a score is attributed to the data source considering the following indicators: reliability, completeness, temporal, geographical, further technological correlation and sample size. Additionally, the indicator 'basic uncertainty' is

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[49] https://www.greenscreenchemicals.org/learn/full-greenscreen-method (accessed on 14/04/2022)

[50] This discussion assumes the evaluation output is a rating level, but it applies equally to the case in which the output is a cardinal value on an interval scale.

considered to account for intrinsic variability and stochastic error of the data. Also, a general requirement for data sources used for the SSbD assessment is that they provide data in a findable, accessible, interoperable and reusable (FAIR) format.

To support these, additional data-related criteria are necessary, ensuring that relevant and high-quality data is used for the assessments. Links to other data initiatives are therefore necessary, including the adoption of FAIR (findable, accessible, interoperable and reusable) data principles (Wilkinson et al. 2016; Jeliazkova et al., 2021) and implementation of data quality systems and models already in place (see for example Basei et al., 2022; Furxhi et al., 2022). Generally, such criteria refer to data completeness and data quality (Robinson et al., 2016) that look at availability of (meta) data, usefulness, clarity and correctness of data and datasets. The inclusion of FAIR data principles should in any case substantially improve the reliability of the SSbD assessment performed.

This information should be reflected in the scoring system. A scalable data quality is also conceivable, i.e. on the individual (aspects) level, on the more general dimension level or on the overall SSbD concept level.

These options will be further discussed and tested in the case studies in order to select the most appropriate solution for the SSbD evaluation.

7. Conclusions

This report proposes a framework, developed in the context of the Chemicals Strategy for Sustainability, to define safe and sustainable by design (SSbD) criteria for chemicals and materials, including approaches for setting an evaluation procedure that allows the identification of SSbD chemicals and materials. The framework proposed was build based on underpinning principles that stemmed from consultation with experts and feedback from stakeholders. By providing guidance on how to develop criteria for 'safe' and 'sustainable' chemicals/materials, the framework aims at steering innovation towards the green industrial transition, substituting or minimising the production and use of substances of concern and minimising the impact on climate and the environment along the chemical/material life cycle, considering its functionality.

The framework adopts a hierarchical approach in which safety aspects are considered first, followed by environmental, social and economic aspects. It entails a (re)design phase in which design guiding principles are proposed to support the design of chemicals and materials, and a safety and sustainability assessment phase in which the safety, environmental and socio-economic sustainability of the chemical/material is assessed. The safety and sustainability assessment is constituted of five steps. The first three steps assess safety aspects such as hazard properties (Step 1), human health aspects in the chemical/material production and processing phase (Step 2), human health and environmental effects in the application phase (Step 3). Step 4 assess impacts along the entire chemical/material life cycle, and Step 5 explores aspects that in the future can be used to assess socio-economic dimensions.

The suggestions for the definition of criteria proposed in the report consider the application of different approaches/methodologies that will be further explored in its application to case studies. This will allow to evaluate if any overlap of aspects covered among the different steps, mapping underpinning data used in each of them, and identify limitations in its application. This will allow to identify data gaps as well as research needs that can in the future be addressed in initiatives by the Commission.

A transparent assessment process supported by FAIR data as well as data generated using NAMs, along the entire life cycle of the chemical or material, should be prioritised and included as much as possible in the case studies demonstration and future implementations. The quality and availability of data has shown to be the determining factor to identify the appropriate approach for the assessment of each of the steps of the framework. Thus, additional data quality criteria as well as minimum data (information) requirements need to be defined and implemented to complement the SSbD criteria, ensuring that relevant and high-quality data is used for the sustainability assessment.

The next step will include a testing phase for the SSbD framework (e.g. case studies covering several types of chemicals or materials) that should support further refinement of the framework and advance on SSbD criteria definition. Thus, additional and clearer conclusions on the applicability of the framework will be drawn after the case study and testing phase, where the aspects and indicators will be optimised for the specific cases and needs.

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List of Abbreviations

AE	Accumulated Exceedance
AESA	Absolute Environmental Sustainability Assessment
AI	Artificial Intelligence
BREFs	Best Available Techniques Reference
CC	Circular Chemistry (principles)
CFC-11	Trichlorofluoromethane (Freon-11 and R-11)
COSHH	Control of Substances Hazardous to Health
CLP	Classification, labelling and packaging of substances and mixtures (Regulation (EC) N. 1272/2008)
CRM	Critical Raw Material
CSS	Chemicals Strategy for Sustainability
CTUh	Comparative Toxic Unit for humans
CV	Control Variables
DEX	Decision EXpert
DRSA	Dominance based Rough Set Approach
DG RTD	Directorate General for Research and Innovation
EC	European Commission
ECHA	European Chemicals Agency
ED	Endocrine Disruptor / Disruption
EF	Environmental Footprint
ELoC	Equivalent level of concern
ERCs	Environmental Release Categories
FAIR	Findable, Accessible, Interoperable and Reusable
GC/GCP	Green Chemistry Principles
GE/GEP	Green Engineering Principles
GHG	Greenhouse gases
GLAM	Global Guidance for Life Cycle Impact Assessment Indicators and Methods
GR	Golden Rules
GRI	Global Resource Indicator
GWP	Global Worming Potential
IPCC's	Intergovernmental Panel on Climate Change
JRC	Joint Research Centre
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCSA	Life Cycle Sustainability Assessment
LCT	Life Cycle Thinking
LCIA	Life Cycle Impact Assessment
MCDA	Multiple-criteria Decision Analysis
MCI	Material Circularity Indicator

ML	Machine Learning
MVCs	Monetary Value Coefficients
N	Nitrogen
NALD	Non-Aqueous Liquid Discharge
NAMs	New Approach Methodologies
NBL	Natural occurring background level
NMVOC	Non-methane volatile organic compounds
NRC	National Research Council
ODP	Ozone Depletion Potential
OSH	Occupational safety and health
O_3	Ozone
P	Phosphorus
PB	Planetary Boundary
PBT/vPvB	Persistent, bioaccumulative and toxic / very persistent and very bioaccumulative
PEC	Predicted Environmental Concentration
PEF	Product Environmental Footprint
PEFCR	Product Environmental Footprint Category Rules
PM	Particulate Matter
PMT/vPvM	Persistent, mobile and toxic / very persistent and mobile
PNECs	Predicted No-effect Concentrations for the Environment
PVC	Polyvinyl Chloride
R&D	Research and Development
RRI	Responsible Research and Innovation
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals (Regulation (EC) N. 1907/2006)
RMMs	Risk Management Measures
Sb eq	Equivalents of kilograms antimony
SbD	Safe by Design
SC	Sustainable Chemistry (principles)
SDGs	Sustainable Development Goals
SDS	Safety Data Sheet
SIA	Safe Innovation Approach
SIRs	Standard information requirements
S-LCA	Social Life Cycle Assessment
SME	Small and Medium Enterprises
SOS	Safe Operational Space
SpERCs	Specific Environmental Release Categories
SPI	Sustainable Products Initiative
SSbD	Safe and Sustainable by Design

SSD	Species Sensitivity Distributions
SSBDCHEM	Safe and Sustainable by Design advanced materials and chemicals
STOT-SE	Specific target organ toxicity – single exposure
STOT-RE	Specific target organ toxicity - repeated exposure
SVHC	Substance of Very High Concern
TRL	Technology Readiness Level
U235	Uranium 235
VRE	Value-based resource efficiency indicator
WMO	World Meteorological Organisation
WoE	Weight of Evidence

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Annexes

Annex 1. Definitions

Term	Definition	References (*if applicable*)
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	EU (2006). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 Concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (OJ L 396 30.12.2006).
Aspect	Refers to an element of an organisation's activities, products or services that interacts or can interact with the environment/ society/ economy	ISO (2015). ISO 14001:2015 Environmental management systems - Requirements with guidance for use
Characterisation factor	Factor derived from a characterisation model which is applied to convert an assigned life cycle inventory analysis result to the common unit of the impact category indicator	ISO (2006). ISO 14040:2006 Environmental management — Life cycle assessment — Principles and framework
Chemicals	Substances and mixtures as defined in REACH	
Chemical Pollution	Emissions, concentrations, or effects on ecosystem and Earth System functioning of persistent organic pollutants, plastics, endocrine disruptors, heavy metals, and nuclear wastes	Rockström et al. (2009a) Planetary Boundaries: Exploring the Safe Operating Space for Humanity. Ecology and Society. 14(2): 32.
Chemical product	(Chemical product or a material product) - a chemical or material intended for consumers or that is likely -under reasonably foreseeable conditions- to be used by consumers	EC (2021e). Mapping Study for the Development of Sustainable-by-Design Criteria.
Criteria	An aspect with an assessment method and a minimum threshold or target values (on which a decision may be based)	
Decision Framework	The decision structure made of principles, methods, and indicators to proceed from the relevant information to final outcomes that are necessary to inform future actions. The collected frameworks can be either recommended by experts in guidance documents and articles or implemented in design tools.	

Term	Definition	References (*if applicable*)
Endpoint (Risk Assessment)	An observable or measurable inherent property of a chemical substance. It can for example refer to a physical-chemical property like vapour pressure or to degradability or a biological effect that a given substance has on human health or the environment, e.g. carcinogenicity, irritation, aquatic toxicity.	EU (2006). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 Concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (OJ L 396 30.12.2006). https://echa-term.echa.europa.eu/ (Retrieved November 16, 2021)
Endpoint method-model and indicator (LCA)	The category endpoint is an attribute or aspect of the environment, human health, or resources, identifying an environmental issue giving cause for concern. Hence, endpoint method (or damage approach)/model) is a characterisation method/model that provides indicators at the level of Areas of Protection (natural ecosystems, human health, resource availability) or at a level close to the Areas of Protection level.	ISO (2006). ISO 14040:2006 Environmental Management - Life Cycle Assessment - Principles and Framework.
Environmental cause-effect chain	Also known as an environmental mechanism. System of physical, chemical and biological processes for a given impact category, linking the life cycle inventory analysis result to the common unit of the category indicator (ISO 14040) by means of a characterisation model.	ISO (2006). ISO 14040:2006 Environmental Management - Life Cycle Assessment - Principles and Framework.
Environmental pressure	The quantified cause of a change to the environment	
Exposure	Contact of an organism with a chemical, radiological, or physical agent. Exposure is quantified as the amount of the agent available at the exchange boundaries of the organism (e.g. skin, lungs, gut) and available for absorption. The chemical safety assessment shall be based on a comparison of the potential adverse effects of a substance with the known or reasonably foreseeable exposure of man and/or the environment to that substance taking into account implemented and recommended risk management measures and operational conditions.	https://echa-term.echa.europa.eu/ (Retrieved November 16, 2021)
	Concentration or amount of a particular substance that is taken in by an individual, population or ecosystem in a specific frequency over a certain amount of time.	EFSA Glossary https://www.efsa.europa.eu/en/glossary-taxonomy-terms (Retrieved January 27, 2022)
Framework	The rationale and the structure for the identification of sustainability dimensions as well as the way to integrate concepts, parameters, methodologies, methods, models, tools and indicators.	Sala, S., Farioli, F., Zamagni, A. (2013). “Progress in Sustainability Science: Lessons Learnt from Current Methodologies for Sustainability Assessment: Part 1.” International Journal of Life Cycle Assessment 18, 9, 1653–72. https://doi.org/:10.1007/s11367-012-0508-6.
Hazard	A substance or activity which has the potential to cause adverse effects to living organisms or environments	EFSA Glossary https://www.efsa.europa.eu/en/glossary-taxonomy-terms (Retrieved November 16, 2021)
	Property or set of properties that make a substance dangerous	REACH (EC 1907/2006); https://echa-term.echa.europa.eu/ (Retrieved November 16, 2021)
Impact	The quantified result of a change to the environment caused by human activity that can be positive or negative	

Term	Definition	References (*if applicable*)
Impact category	Class representing environmental issue of concern, e.g. climate change, acidification, ecotoxicity etc.	ISO (2006). ISO 14040:2006 Environmental Management - Life Cycle Assessment - Principles and Framework.
In silico methods	Computer-based approaches (often called non-testing methods). They can be used to efficiently and effectively predict the toxicology of chemicals directly from their basic properties such as their structure, for example.	EU Science Hub, EURL ECVAM FAQ https://ec.europa.eu/jrc/en/eurl/ecvam/faq/general (Retrieved November 23, 2021)
In vitro test methods	These methods use tissues, reconstructed tissues, whole cells or parts of cells. Recent advances in cell-based research include the two and three dimensional cell cultures which mimic very closely cells and tissues in the human body.	EU Science Hub, EURL ECVAM FAQ https://ec.europa.eu/jrc/en/eurl/ecvam/faq/general (Retrieved November 23, 2021)
In vivo testing	Testing within a living organism.	https://echa-term.echa.europa.eu/ (Retrieved November 23, 2021)
Indicator	A parameter, or a value derived from parameters, which points to, provides information about, or describes the state of a phenomenon, with a significance extending beyond that directly associated with its value (OECD 2003). The indicator could be quantitative or semi- quantitative or qualitative derived from a model, often trough a tool or direct measurement	Adapted from OECD, OECD. 2021. Glossary of statistical terms. Retrieved November 16, 2021 (https://stats.oecd.org/glossary/detail.asp?ID=830)
Life cycle assessment	Methodology for assessing life cycle impacts standardised by ISO 14040:2006 and ISO 14044:2006	ISO (2006). ISO 14040:2006 Environmental Management - Life Cycle Assessment - Principles and Framework.
Life cycle thinking	Life Cycle Thinking (LCT) is about going beyond the traditional focus on production site and manufacturing processes to include environmental, social and economic impacts of a product over its entire life cycle. The main goals of LCT are to reduce a product's resource use and emissions to the environment as well as improve its socio-economic performance through its life cycle.	https://www.lifecycleinitiative.org/starting-life-cycle-thinking/what-is-life-cycle-thinking/
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 (EC 2021c).	EC (2021b). Sustainable products initiative. https://ec.europa.eu/info/law/better-regulation/have-your-say/initiatives/12567-Sustainable-products-initiative_en (accessed 11.16.21).
Measurement	Direct measurement of a certain aspect following a procedure	
Methodology	A collection of individual methods, which together address the different safety, environmental, economic and social issues and the associated effect/ impact (e.g. risk assessment, LCA, LCC, sLCA….)	
Method	A procedure for measurement or a set of models, tools and indicators that enable the calculation of indicators' values for a certain parameter	
Midpoint method and indicator (LCA)	In LCA, the midpoint method is a characterisation method that provides indicators for comparing environmental interventions at the level of a cause-effect chain between emissions/resource consumption and the endpoint level (where effects and damage are assessed)	

Term	**Definition**	**References** (*if applicable*)
Mixture	A mixture or solution composed of two or more substances	EU (2006). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 Concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (OJ L 396 30.12.2006).
Model	A model supporting the quantitative assessment of safety/environmental/social/economic parameters adopted in order to calculate a particular indicator	
Parameter	Refers to a value, a constant, as a mathematical term. In environmental science and particularly in chemistry and microbiology, a parameter is used to describe a discrete chemical or microbiological entity that can be assigned a value.	
Product	Any goods or services which are supplied for distribution, consumption or use on the Community market whether in return for payment or free of charge	EU (2010). Regulation (EC) No 66/2010 of the European Parliament and of the Council of 25 November 2009 on the EU Ecolabel. OJ L 27, 30.1.2010, p. 1–19
Product design	'Product design' means the set of processes that transform legal, technical, safety, functional, market or other requirements to be met by a product into the technical specification for that product.	EU (2009). Directive 2009/125/EC of the European Parliament and of the Council of 21 October 2009 Establishing a Framework for the Setting of Ecodesign Requirements for Energy-Related Products.
Safety	The responsibility of protecting from harm or other psychophysical dangers	
Safe and sustainable-by-design	A pre-market approach to chemicals that focuses on providing a function (or service), while avoiding volumes and chemical properties that may be harmful to human health or the environment, in particular groups of chemicals likely to be (eco) toxic, persistent, bio-accumulative or mobile. Overall sustainability should be ensured by minimising the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity from a life cycle perspective	EC (2020a). Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee and The Committee of the Regions - Chemicals Strategy for Sustainability - Towards a Toxic-Free Environment COM (2020) 667
Safe-by-Design, Safer-by-Design, or Safety-by-Design	The concept refers to identifying the risks and uncertainties concerning humans and the environment at an early phase of the innovation process so as to minimise uncertainties, potential hazard(s) and/or exposure. The SbD approach addresses the safety of the material/product and associated processes through the whole life cycle: from the Research and Development (R&D) phase to production, use, recycling and disposal.	OECD (2020). Moving Towards a Safe(r) Innovation Approach (SIA) for More Sustainable Nanomaterials and Nano-Enabled Products.
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	EU (2006). Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 Concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (OJ L 396 30.12.2006).
Sustainability dimensions	Refers to the four dimensions of sustainability addressed in this study: safety, environmental, social and economic	

Term	**Definition**	**References** (*if applicable*)
Tool	Software, applications, databases supporting the analysis done by adopting specific methods and the related models (e.g. a software for LCA calculation, or a QSAR tool)	

Annex 2. Principles to support the development of SSbD chemicals and materials

The concept of safe and sustainable chemicals and materials implies to minimise the emission of pollutants into environment and the use of natural resources with the aim of reducing the negative impacts to human and ecosystems health. This perspective can be considered during the design phase of a chemical/material and the design of its manufacturing process using several strategies which include, for example, increasing the process efficiency in terms of energy and material, applying the waste hierarchy (reduce-reuse-recycle), using innovative business models, looking for industrial symbiosis (Corona, et al. 2019). Many of these approaches are underpinned by the Green Chemistry and Green Engineering principles (Table A2.1-2), which are the cornerstone of Sustainable Chemistry and can be used to improve the safety and sustainability performance of chemicals and materials. Other relevant guidelines on this topic are the Sustainable Chemistry and the Golden Rules criteria developed by UBA (UBA, 2009; 2016), which also take into account the use of LCA as a comprehensive method for assessing sustainability. Note that these principles and rules cover in some cases the same elements. We, nevertheless, report them all.

Table A2.1 List of Green Chemistry Principles (from Anastas and Warner, 1998).

Green Chemistry Principles (GCP)
1 - Prevention
2 - Atom Economy
3 - Less Hazardous Chemical Syntheses
4 - Design Safer Chemicals
5 - Safer Solvents and Auxiliaries
6- Design for Energy Efficiency
7 - Use of Renewable Feedstock
8 - Reduce derivatives
9 - Catalysis
10 - Design for Degradation
11 - Real-time analysis for Pollution Prevention
12 - Inherently Safer Chemistry for Accident Prevention

Table A2.2 List of Green Engineering Principles (from Anastas and Warner, 2003).

Green Engineering Principles (GEP)
1 - Inherent rather than Circumstantial
2 - Prevention Instead of Treatment
3 - Design for Separation
4 - Maximise Efficiency
5 - Output-Pulled Versus Input-Pushed
6 - Conserve Complexity
7 - Durability Rather than Immortality

8 - Meet Need, Minimise Excess
9 - Minimise Material Diversity
10 - Integrate Material and Energy Flows
11 - Design for commercial “Afterlife”
12 - Renewable rather than Depleting

Table A2.3 List of Circularity Principles (from Keijer et al. 2019).

	Name	**Description**
CC1	Collect and use waste.	Waste is a valuable resource that should be transformed into marketable products.
CC2	Maximise atom circulation.	Circular processes should aim to maximise the utility of all atoms in existing molecules.
CC3	Optimise resource efficiency.	Resource conservation should be targeted, promoting reuse and preserving finite feedstocks.
CC4	Strive for energy persistence	Energy efficiency should be maximised.
CC5	Enhance process efficiency.	Innovations should continuously improve in- and post-process reuse and recycling, preferably on-site.
CC6	No out-of-plant toxicity.	Chemical processes should not release any toxic compounds into the environment.
CC7	Target optimal design	Design should be based on the highest end-of-life options, accounting for separation, purification and degradation.
CC8	Assess sustainability.	Environmental assessments (typified by the LCA) should become prevalent to identify inefficiencies in chemical processes.
CC9	Apply ladder of circularity.	The end-of-life options for a product should strive for the highest possibilities on the ladder of circularity.
CC10	Sell service, not product.	Producers should employ service-based business models such as chemical leasing, promoting efficiency over production rate.
CC11	Reject lock-in.	Business and regulatory environment should be flexible to allow the implementation of innovations.
CC12	Unify industry and provide coherent policy framework	The industry and policy should be unified to create an optimal environment to enable circularity in chemical processes.

Criteria for Sustainable Chemistry (UBA, 2009)

Accordingly, the general principles refer to the need of using comprehensive LCAs in order to reduce the consumption of resources and energy and to avoid the use of dangerous substances. Additional principles refer to the:

- 'use of harmless substances, or where this is impossible, substances involving a low risk for humans and the environment, and manufacturing of long-life products in a resource-saving manner;
- reduction of the consumption of natural resources, which should be renewable wherever possible, avoidance or minimisation of emission or introduction of chemicals or pollutants into the environment. Such measures will help to save costs;
- avoidance, already at the stage of development and prior to marketing, of chemicals that endanger the environment and human health during their life cycle and make excessive use of the environment as a source or sink; reduction of damage costs and the associated economic risks for enterprises and remediation costs to be covered by the state; and
- the need for economic innovation: sustainable chemicals, products and production methods produce confidence in industrial users, private consumers, and customers from the public sector and thus, result in competitive advantages.

UBA golden rules (UBA, 2016)

Rule 1- If possible, only use substances (as such, in mixtures or in articles) which are not mentioned on lists of problematic substances! This way you avoid losing raw materials because of legitimate restrictions.

Rule 2- In the case of using problematic substance, it should be assessed the different uses and potential users of the substance as such. If the substance cannot be substituted, you have to take responsibility for the consequences of its use. Never only evaluate the substance in isolation but think through the entire lifecycle!

Rule 3- As much as possible use substances which are not dangerous to human health (in particular none, which are classified as carcinogenic, mutagenic or reprotoxic), which are easily degraded, don't bioaccumulate and don't widely disperse in the environment! With these substances you have to put less effort in risk management measures.

Rule 4- Don't use substances which require a high degree of risk management according to the easy-to-use workplace control scheme for hazardous substances or the COSHH (Control of Substances Hazardous to Health) approach!

Rule 5- Prefer substances which are available in excess or made from renewable resources to substances which are scarce and produced from fossil raw materials! On the one hand, you will pay less for them. On the other, they will probably still be available for you in 20 years.

Rule 6- Avoid long-distance transports at any stage of the supply chain, in particular for substances which you use in high amounts! Transport always correlates with higher environmental stress.

Rule 7- Pay attention to a low energy and water consumption of substances you use in large amounts as well as to a low generation of wastes in manufacturing and use! That way you conserve limited resources.

Rule 8- Assess whether your suppliers conform to high environmental and social standards. Select substances considering the transparency of the supply chain and the commitment of its actors to sustainability! That is how you support enterprises that do their responsibility in the supply chain justice.

Rule 9- Furthermore, products should not be put on the market for which a societal benefit and a benefit for consumers can not be identified.

The principles/rules abovementioned are examples of relevant considerations to take into account in the design phase of a chemical/material or in the redesign of its production process that can lead to a better safety and sustainability performance. The chemical/material developer might consider pinpointing to which principles/rules it has adhered to provide as additional information to the assessment. As mentioned, the safety, environmental and socio-economic sustainability of the chemicals and materials designed following these principles should be verified, namely assessing the extent to which they comply with specific safe and sustainability criteria.

These principles/rules can be translated in indicators, as the ones provided below (Table A2.4) that can be used to depict characteristics of the chemical/material system. These indicators are not to be used in the assessment but only as additional information to help guide the chemical/material design.

As pointed out in Figure 9, the SSbD process can be iterative. If the current chemical/material does not meet the minimum of SSbD criteria, then the company could go back to design phase and make improvements. To reduce the effort needed for the assessment of Step 1 to 4, these indicators could be used and helpful (e.g. in screening several preliminary alternative design).

Below (Table A2.4) are reported the indicators suggested in section 4.1 along with their area of intervention, their definition and the relative assessment method for each indicator. It has to be remarked that these indicators are examples being proposed. Other indicators or information not reported in this document can be used.

Table A2.4: Indicators to be used to guide the design: definition and assessment method

Areas of Intervention	Indicator	Definition	Assessment Method
Resource/ feedstock	Net mass of materials consumed (kg/kg)	Use of raw materials for the manufacturing of the chemical/materials produced, along the life cycle.	Curzons et al., 2007
	Material intensity index (%)	Ratio between the kg of raw materials used per kg of chemical or material produced.	Calculated according to Cervera-Padrell et al., 2012.
	Critical raw materials presence (yes/no)	Use of materials that are present in the list of critical raw materials in the chemical/material manufacturing and supply-chain.	Critical Raw Materials as listed at: https://ec.europa.eu/growth/sectors/raw-materials/specific-interest/critical_en
	Recycled content (%)	Percentage of recycled content in the chemical or material.	Measurement
	Water consumption (m^3/kg)	Net amount of water consumed by a process, product or system per unit of chemical/material produced.	Establish a water balance measuring all the water withdrawn and discharge from the organisation site.
	Value-based resource efficiency indicator (VRE)	Measure resource efficiency and circular economy in terms of the market value of 'stressed' resources (i.e., this value includes elements of scarcity versus competition as well as taxes representing urgent social and environmental externalities) to produce a certain material or chemical. Therefore, it may be a suitable indicator to monitor, steer and manage the performance of actors in the supply/value chain and, thus, the total supply/value chain.	Calculated according to Di Maio et al., 2017
	Energy consumption (kWh/kg or MJ/kg)	Measure of the energy consumed by a process or system per unit of chemical/material produced.	Calculated with real plant data or estimated at design level.
	Energy efficiency (%)	Ratio between the energy produced and the energy carrier input.	Calculated with real plant data or estimated at design level.
	Renewable or fossil feedstock? (yes/no)	Origin of the feedstock/energy i.e. fossil or renewable.	Type of feedstock/energy used to be reported
	Share of Renewable Energy (%)	The indicator is assessed as percentage of renewable energy resources over total energy used in the manufacturing process (gate-to-gate). This indicator accounts for energy resources from fossil, nuclear, hydro, biomass and solar, wind and geothermal source.	Calculated with real plant data or with the use of supplier specific energy mix or national residual mix.

Areas of Intervention	Indicator	Definition	Assessment Method
	Classification of raw chemicals/materials as SVHC (yes/no)	Report if the manufacturing process of the chemical/material use substances from the candidate list of substances of very high concern.	Check the chemicals/materials according to REACH (EC No 1907/2006).
Process efficiency	Atom economy (%)	Conversion efficiency of a chemical reaction in terms of all atoms involved and the desired products produced according to stoichiometry.	Calculated with plant real data or estimated at design level. E.g. Trost, 1991.
	Reaction yield (%)	Yield or of a biochemical or thermochemical reaction, calculated as the amount of produced chemical divided by the amount of theoretical maximum amount according to stoichiometry.	Calculated with plant real data or estimated at design level
	Yield of extraction (%)	Yield or efficiency of a thermochemical extraction process aiming at recycling a solvent calculated as the amount of recovered chemical divided by the amount of chemical present before the separation.	Calculated with plant real data or estimated at design level.
	Boiling temperature (°C)	Boiling temperature is used as a proxy for easiness to be recycled (since often the recycling is done via distillation). It can be used to as a criteria for selection of solvents in the manufacturing process of the chemical/material.	Literature or experimental data
	Heat of vaporisation (MJ/kg)	Heat of vaporisation is used as a proxy for the energy required for recycling this substance (since often the recycling is done via distillation). It can be used to as a criteria for selection of solvents in the manufacturing process of the chemical/material.	Literature or experimental data
	Solvent selectivity [-]	The ability of a given solvent to selectively dissolve one compound as opposed to another. It can be used to as a criteria for selection of solvents in the manufacturing process of the chemical/material.	Literature or experimental data
Emissions	Biological oxygen demand (g/kg)	Measure of the amount of oxygen consumed by microorganisms while they decompose organic matter under aerobic (oxygen is present) conditions at a specified temperature i.e. 5 days of incubation at 20 °C. Calculated as the total oxygen demand (in mass) of the released wastewater per unit of chemical/material produced.	Calculated according to e.g. Sawyer et al., 2003
	Chemical oxygen demand (g/kg)	Measure of the amount of oxygen that can be consumed by reactions in a measured solution. Calculated as the total oxygen demand (in mass) of the released wastewater per unit of chemical/material produced.	Calculated according to e.g. Sawyer et al., 2003
	Total organic carbon (g/kg)	Total soluble and insoluble organic matter going into water bodies. Calculated as the total oxygen demand (in mass) of the released wastewater per unit of chemical/material produced.	Calculated according to Goerlitz and Brown., 1972
	Critical air mass (%)	Indicator representing the mass of air emissions over a standard value (maximum acceptable amount of pollutants).	Calculated according to e.g. Stefanis et al., 1996

Areas of Intervention	Indicator	Definition	Assessment Method
	Critical water mass (%)	Indicator representing the mass of water emissions over a standard value (maximum acceptable amount of pollutants).	Calculated according to e.g. Stefanis et al. (1996)
Waste	Non-Aqueous Liquid Discharge (m^3/kg)	Amount of (non-aqueous) liquid waste produced per kg of chemical/material. Further developments of this aspect may come from the sustainable waste management strategy, Zero Liquid Discharge, which allows recovering and reuse non-aqueous waste by applying novel technologies (e.g. membrane technology) which are less energy intensive than existing ones (e.g. distillations).	Calculated with plant real data or estimated at design level. Note that for the EU taxonomy (Platform on Sustainable Finance, 2022a,b) of investments, the solvents loss from total inputs cannot exceed 3%.
	E-factor (%)	The ratio between mass of waste per mass of chemical/material.	Calculated with plant real data or estimated at design level. See Sheldon (2017)
	Wastewater to treatment (m^3/kg)	The quantity of wastewater sent to wastewater treatment outside of the organisation, or released into water bodies, per unit of chemical/material manufactured.	Calculated with plant real data or estimated at design level
	Total amount of waste (kg waste/kg)	Mass of waste generated e.g. solid, liquid waste or wastewater per unit of chemical/material.	Calculated with plant real data or estimated at design level
	Amount of waste to landfill (kg waste/kg of chemical)	The quantity of industrial waste disposed in a landfill, per kg of chemical/material.	Calculated with plant real data or estimated at design level
	Amount of hazardous waste (kg waste/kg)	The quantity of hazardous waste generated in the manufacturing process per unit of mass of chemical/material.	Calculated with plant real data or estimated at design level.
	Recyclable? (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.
	Recycling efficiency/recovery 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.
	Material Circularity Indicator (MCI)	Measures the extent to which linear flows have been minimised and restorative flows maximised for the component materials of a chemical or material, and for how long and intensively the materials are used compared to a similar industry-average product. The result is a value between 0 and 1.	Calculated according to e.g. EMF and Granta (2019)
	Purity of recovered solvent (%)	Percentage of purity of the solvent obtained from the recycling process.	Calculated with plant real data or estimated at design level.

Areas of Intervention	Indicator	Definition	Assessment Method
Characteristics of the chemical/material	Biodegradability of manufactured chemical/material (yes/no)	Ability of a chemical/material to decompose after interactions with biological elements.	Calculated according to e.g. Arnot et al. (2008a,b)
	Disassembly/reparability design (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).	[-]
	Durability (years)	Measurement of how long the chemical/material may last, while performing its function.	Real data from testing or estimated at design level.

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Annex 3. GHS Column Model

The GHS Column Model developed by the Institute for Occupational Safety and Health of the German Social Accident Insurance (IFA, 2020), groups several aspects especially related to the acute human health hazards, physical hazards and other specific process-related aspects. For chronic health hazards, the groups defined in Step 1 of the framework has been used in order to not introduce another system of evaluating severity of hazards and keep align the two steps.

The Column Model was developed primarily to support the substitution assessment regarding hazardous substances, but the approach could also be adapted for other purposes and by using the same information already collected.

The approach allows the assessment of the production process based on the following aspects (Table A3.1):

- Acute human health hazards
- Chronic human health hazards
- Physical properties
- Hazards from release behaviour
- Process-related hazards

The information needed (e.g. the hazards statements) for the assessment could be extracted from the Safety Data Sheet (SDS), available for each substance used in the process.

Table A3.1. List of aspects and indicators relevant for Step 2

Group definition	Acute human health hazards*	Chronic human health hazards	Physical properties*	Hazards from release behaviour*	Process-related hazards*
Aspects related to <u>very high-risk process</u>	• Acutely toxic substances/mixtures, Cat. 1 or 2 (H300, H310, H330) • Substances/mixtures that in contact with acids liberate highly toxic gases (EUH032)	• Human hazards similar to Step 1 / Criterion H1 (Table 3).	• Instable explosive substances/mixtures (H200) • Explosive substances/mixtures/articles, divisions 1.1 (H201), 1.2 (H202), 1.3 (H203), 1.4 (H204), 1.5 (H205) and 1.6 (without H-phrase) • Flammable gases, Cat. 1A (H220, H230, H231, H232) and Cat. 1B and 2 (H221) • Pyrophoric gases (H232) • Flammable liquids, Cat. 1 (H224) • Self-reactive substances/mixtures, Types A (H240) and B (H241) • Organic peroxides, Types A (H240) and B (H241) • Pyrophoric liquids or solids, Cat. 1 (H250) • Substances/mixtures which in contact with water emit flammable gases, Cat. 1 (H260) • Oxidising liquids or solids, Cat. 1 (H271)	• Gases • Liquids with a vapour pressure > 250 hPa (mbar) • Dust-generating solids • Aerosols	• Open processing • Possibility of direct skin contact • Large-area application • Open design or partially open design, natural ventilation
Aspects related to <u>high-risk process</u>	• Acutely toxic substances/mixtures, Cat. 3 (H301, H311, H331) • Substances/mixtures toxic in contact with eyes (EUH070) • Substances/mixtures that in contact with water or acids liberate toxic gases (EUH029, EUH031) • Substances/mixtures with specific target organ toxicity (single exposure), Cat. 1: Organ damage (H370)	• Human hazards similar to Step 1 / Criterion H2 (Table 3).	• Aerosols, Cat. 1 (H222 and H229) • Flammable liquids, Cat. 2 (H225) • Flammable solids, Cat. 1 (H228) • Self-reactive substances/mixtures, Types C and D (H242) • Organic peroxides Types C and D (H242) • Self-heating substances/mixtures Cat. 1 (H251)	• Liquids with a vapour pressure 50 - 250 hPa (mbar)	• Partially open design, process related opening with simple extraction, open with simple extraction

Group definition	Acute human health hazards*	Chronic human health hazards	Physical properties*	Hazards from release behaviour*	Process-related hazards*
	• Skin sensitising substances/mixtures (H317, Sh) • Substances/mixtures that sensitise the respiratory organs (H334, Sa) • Substances/mixtures corrosive to the skin, Cat. 1, 1A (H314)		• Substances/mixtures which in contact with water emit flammable gases, Cat. 2 (H261) • Oxidising gases, Cat. 1 (H270) • Oxidising liquids or solids, Cat. 2 (H272) • Desensitised explosives, Cat. 1 (H206) and Cat. 2 (H207) • Substances/mixtures with certain properties (EUH001, EUH014, EUH018, EUH019, EUH044)		
Aspects related to <u>medium-risk process</u>	• Acutely toxic substances/mixtures, Cat. 4 (H302, H312, H332) • Substances/mixtures with specific target organ toxicity (single exposure), Cat. 2: Possible organ damage (H371) • Substances/mixtures corrosive to the skin, Cat. 1B, 1C (H314) • Eye-damaging substances/mixtures (H318) • Substances/mixtures with corrosive effect on respiratory organs (EUH071) • Nontoxic gases that can cause suffocation by displacing air (e.g. nitrogen)	• Human hazards similar to Step 1 / Criterion H3 (Table 3), except those listed under “acute human health hazards” (left column).	• Aerosols, Cat. 2 (H223 and H229) • Flammable liquids, Cat. 3 (H226) • Flammable solids, Cat. 2 (H228) • Self-reactive substances/mixtures, Types E and F (H242) • Organic peroxides, Types E and F (H242) • Self-heating substances/mixtures, Cat. 2 (H252) • Substances/mixtures which in contact with water emit flammable gases, Cat. 3 (H261) • Oxidising liquids or solids, Cat. 3 (H272) • Gases under pressure (H280, H281) • Corrosive to metals (H290) • Desensitised explosives, Cat. 3 (H207) and Cat. 4 (H208)	• Liquids with a vapour pressure 10 - 50 hPa (mbar), with the exception of water	• Closed processing with possibilities of exposure, e.g. during filling, sampling or cleaning • Closed design, tightness not ensured, partially open design with effective extraction
Aspects related to <u>low-risk process</u>	• Skin-irritant substances/mixtures (H315) • Eye-irritant substances/mixtures (H319)	• Substances chronically harmful in other ways (no H-phrase)*	• Aerosols, Cat. 3 (H229 without H222, H223) • Not readily flammable substances/mixtures (flash	• Liquids with a vapour pressure 2 - 10 hPa (mbar)	• Closed design, tightness ensured, partially closed design with integrated extraction, partially open

Group definition	Acute human health hazards*	Chronic human health hazards	Physical properties*	Hazards from release behaviour*	Process-related hazards*
	• Skin damage when working in moisture • Substances/mixtures with a risk of aspiration (H304) • Skin-damaging substances/mixtures (EUH066) • Substances/mixtures with specific target organ toxicity (single exposure), Cat. 3: irritation of the respiratory organs (H335) • Substances/mixtures with specific target organ toxicity (single exposure), Cat. 3: drowsiness, dizziness (H336)		point > 60 … 100 °C, no H-phrase) • Self-reactive substances/mixtures, Type G (no H-phrase) • Organic peroxides, Type G (no H-phrase)		design with highly effective extraction
Aspects related to <u>negligible risk</u>	• Substances of no concern regarding intrinsic hazard properties, according to Step 1 criteria			• Liquids with a vapour pressure < 2 hPa (mbar) • Non-dust-generating solids	

*Adapted from GHS Column Model (version 2020) developed by the Institute for Occupational Safety and Health of the German Social Accident Insurance (IFA, 2020)

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Annex 4. Description of the Environmental Footprint 3.0 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 CO2.

Ozone depletion

The stratospheric ozone (O3) 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 model called USEtox.

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 PM2.5 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. The most significant sources of phosphorus emissions are 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 a model called USEtox.

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 5. Planetary Boundaries

Table A5.1: Overview of the nine Planetary Boundaries (Rockström et al., 2009b; Steffen et al., 2015). For a full description of current control variables (CV), planetary boundaries (CV) and the current value of control variable, read Table 1 in Steffen et al. (2015).

Planetary Boundary	CV	PB	SOS
Climate Change	- Atmospheric CO2 concentration (ppm) - Energy imbalance at top-of-atmosphere (W m^{-2})	350 1	72 1
Biosphere Integrity	- Genetic diversity: extinction rate (E/MSY) - Functional diversity: Biodiversity intactness (% BII loss)	10 10	<10 10
Stratospheric Ozone Depletion	Stratospheric O_3 concentration (DU)	275	15
Ocean Acidification	Carbonate ion concentration (Ωarag)	2.75	0.69
Biochemical Flows	- Phosphorus (P) Global: P flow from freshwater to ocean (Tg P yr^{-1}) , Regional: P flow from fertilizers to erodible soils (Tg yr^{-1}) - Nitrogen (N) Global: biological fixation of N (Tg N yr^{-1}),	 11 6.2 62	 9.9 6.2 62
Land-system change,	- Global: area (%) of original forest cover - Biome: area (%) of potential forest	75 85*	25 15
Freshwater use	- Global: maximum consumptive blue water use (km^3yr^{-1}) - Basin: withdrawal of blue water as percentage of mean monthly river flow (in %)	4000 55**	4000 45
Atmospheric aerosol loading	- Global: atmospheric aerosol loading (AOD) - Regional: seasonal average based on Asian Monsoon case study (AOD)	- 0.25	- 0.10***
Novel Entities (chemical pollution)	Not yet defined	-	-

E/MSY = extinctions per million species-years; BII = Biodiversity Intactness Index; DU = Dobson Units; Ωarag = saturation state of aragonite; AOD = aerosol optical depth. *Tropical: 85%, temperate: 50% and boreal: 85%, changes to temperate forests have a weaker influence on the global climate system than tropical and boreal.
**Depending on low-, intermediate- or high-flow months which are respectively 25%, 30% and 55%.
***Assuming 0.15 AOD as natural background (Steffen et al., 2015)

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Annex 6. Social sustainability aspects and indicators

Table A6.1 List of social aspects included in the frameworks under investigation (o: optional aspects in the WBCSD framework)

Stakeholders	Social aspects	N° of frameworks including the aspect	UNEP 2020	WBCSD 2016	Goedkoop et al., 2020	Caldeira et al. 2022	Platform Sust. Finance 2022c	EC 2017	OECD 2011	CEFIC 2022
WORKERS	Fair salary	8	x	x	x	x	X	x	x	x
	Forced labour	8	x	x	x	x	x	x	x	x
	Health and Safety	8	x	x	x	x	x	x	x	x
	Child labour	8	x	x	x	x	x	x	x	x
	Freedom of association and collective bargaining	7	x	x	x	x	x	x	x	
	Working hours	7	x	o	x	x	x	x		x
	Equal opportunities / discrimination	7	x	o		x	x	x	x	x
	Skills, knowledge and employability	5		x			x	x	x	x
	Social benefits / social security	4	x	o			x			x
	Smallholders including farmers	4	x		x		x			x
	Management of reorganization	3		o				x	x	
	Employment relationships	3	x				x		x	
	Human rights due diligence	3					x	x	x	
	Sexual harassment	2	x			x				
	Working conditions	2				x		x		
	Job satisfaction	2		o						x
	Management of workers individual health	2		o						x
	Noise reduction	1				x				
	Measures to attract women into the workforce or to break down gender segregation in jobs	1					x			
	Pay gap between executives and the average worker not excessive	1					x			
	Implementation of ILO conventions	1						x		
VALUE CHAIN ACTORS (not consumers)	Fair competition	2	x						x	
	Promoting social responsibility	2	x			x				
	Respect of intellectual property rights	2	x						x	
	Supplier relationships	1	x							
	Whealth distribution	1	x							
SOCIETY	Corruption	4	x			x		x	x	
	Prevention and mitigation of armed conflicts	2	x					x		
	Technology development	2	x						x	
	Public commitments to sustainability issues	1	x							
	Contribution to economic development	1	x							

Stakeholders	**Social aspects**	**N° of frameworks including the aspect**	**UNEP 2020**	**WBCSD 2016**	**Goedkoop et al., 2020**	**Caldeira et al. 2022**	**Platform Sust. Finance 2022c**	**EC 2017**	**OECD 2011**	**CEFIC 2022**
	Ethical treatment of animals	1	x							
	Poverty alleviation	1	x							
	Taxation	1							x	
SMALL SCALE ENTREPRENEURS	Meeting basic needs	1			x					
	Access to services and inputs	1			x					
	Women's empowerment	1			x					
	Child labour	1			x					
	Health and safety	1			x					
	Land rights	1			x					
	Trading relationships	1			x					
LOCAL COMMUNITY	Community engagement	6	x	o	x		x	x		x
	Local employment	6	x	x		x	x		x	x
	Safe and healthy living conditions	5	x	x	x				x	x
	Access to material resources (water, minerals, land, biological resources)	4	x	x	x					x
	Respect of indigenous rights	3	x	o			x			
	Access to immaterial resources (e.g. community services, intellectual property rights, freedom of expression, and access to information)	3	x	x						x
	Promotion of skills and knowledge	2		o	x					
	Secure living conditions	2	x							x
	Inclusion of people with disabilities	2					x			x
	Nuisance reduction	1		o						
	Creating and preserving decent jobs	1					x			
	Delocalization and migration	1	x							
	Cultural heritage	1	x							
	Access to basic needs for sustainable development	1		o						
	Contribution to economic development	1			x					
	Access to infrastructure	1					x			
	Child care	1					x			
	Promoting community-driven development	1						x		
	Promoting gender equality	1					x			
	Avoiding and addressing negative impacts on communities affected by business operations	1					x			
CONSUMERS	Health and safety	7	x		x	x	x	x	x	x
	Responsible communication	6			x	x	x	x	x	x
	Consumer privacy	4	x		x		x		x	
	Transparency	3	x						x	x

Stakeholders	Social aspects	N° of frameworks including the aspect	UNEP 2020	WBCSD 2016	Goedkoop et al., 2020	Caldeira et al. 2022	Platform Sust. Finance 2022c	EC 2017	OECD 2011	CEFIC 2022
	Promotion of skills and knowledge	3		o					x	x
	Consumer product experience	2		o				x		
	Accessibility	2			x			x		
	Feedback mechanism	2	x						x	
	Direct impact on basic needs (healthcare, clean water, healthy food, shelter, education)	2		x		x				
	Impact on vulnerable consumers	2						x	x	
	End-of-life responsibility	1	x							
	Affordability	1			x					
	Effectiveness and comfort	1			x					
	Designing products to be durable and repairable	1					x			
	Ensuring access to quality healthcare	1					x			
	Improving access to healthy and highly nutritious food	1					x			
	Improving access to good-quality drinking water	1					x			
	Improving access to good-quality housing	1					x			
	Improving access to education and lifelong learning	1					x			
CHILDREN	Education provided in local community	1	x							
	Health issues for children	1	x							
	Children concerns regarding marketing practices	1	x							

Table A6.2 List of indicators, data sources, aim and approach for the prioritised social aspects (UNEP, 2021b)

Social aspect	Child labour
Aim and approach	The assessment aims to verify if the organization might or is employing children (as defined in the ILO conventions) and to identify the nature of any child labour. It should be looked upon if the conditions are favourable for the occurrence of child labour, and the existence and quality of prevention and mitigating measures taken by the organization.
Suggested indicators	Percentage of working children under the legal age or 15 years old (14 years old for developing economies (%)) Children are not performing work during the night (an example of unauthorized work by the ILO conventions C138 and C182) Records on all workers stating names and ages or dates of birth are kept on file Working children younger than 15 and under the local compulsory age are attending school
Generic data sources (examples)	Childinfo – monitoring the Situation of Children and Women; UNICEF; The International Labour Organisation (ILO), UNICEF and the World Bank initiated the inter-agency research project. Understanding Children's Work (UCW); U.S. Department of Labor
Specific data sources	Interview with directors or human resources officer; interview with workers and trade union representatives; NGO reports; verification of organizations' documents including sustainability reports; interview with local schools and community members.
Social aspect	Fair salary

Aim and approach	This subcategory aims to assess whether practices concerning wages are in compliance with established standards and if the wage provided is meeting legal requirements, whether it is above, meeting, or below industry average and whether it can be considered as a living wage.
Suggested indicators	Lowest paid worker, compared to the minimum wage and/or living wage Number of employees earning wages below poverty line Presence of suspicious deductions on wages Regular and documented payment of workers (weekly, bi-weekly)
Generic data sources (examples)	Generic data source examples • ILO Global Wage Report • Minimum Wage Fixing Convention 1970 (No. 131)
Specific data sources	Country minimum wage; Interview with directors or human resources officer; Verification of organization documents: e.g., wage records; Review of organization-specific reports, such as GRI reports or audit; Interviews with workers; Interview with local NGOs; Review of wage records
Social aspect	Forced labour
Aim and approach	The assessment aims to verify that forced or compulsory labour is not used in the organization.
Suggested indicators	Workers voluntarily agree upon employment terms. Employment contracts stipulate wage, working time, holidays, and terms of resignation. Employment contracts are comprehensible to the workers and are kept on file Birth certificate, passport, identity card, work permit, or other original documents belonging to the worker are not retained or kept for safety reasons by the organization neither upon hiring nor during employment Workers are free to terminate their employment within the prevailing limits Workers are not bonded by debts exceeding legal limits to the employer
Generic data sources (examples)	ILO reports on the advancement of the conventions 29 and 105; U.S. Department of Labor's list of goods produced by child labor or forced labor.
Specific data sources	Interview with directors or human resources officer; verification with workers interviews or audit; NGO reports; verification of organizations' documents.
Social aspect	Health and safety (workers)
Aim and approach	This subcategory aims to assess both the rate of incidents and the status of prevention measures and management practices. An incident is defined as a work-related event in which an injury or ill health (regardless of severity) or fatality occurred or could have occurred.
Suggested indicators	Number/percentage of injuries or fatal accidents in the organization by job qualification inside the company Hours of injuries per level of employees Presence of a formal policy concerning health and safety Adequate general occupational safety measures Preventive measures and emergency protocols exist regarding accidents and injuries Appropriate protective gear required in all applicable situation Number of (serious/non-serious) Occupational Safety and Health Administration (OSHA) violations reported within the past 3 years and status of violations Education, training, counselling, prevention, and risk control programs in place to assist workforce members, their families, or community members regarding serious diseases
Generic data sources (examples)	Generic data source examples • European Agency for Safety and Health at Work • United States Department of Labour – Occupational Safety • World Health Organization • World Health Organization, Harvard School of Public Health, World Bank, Global burden of disease
Specific data sources	Interviews or questionnaire filled out by management, workers, human resources, governmental agencies, NGOs; Review of enterprise-specific reports; Interviews with workers and union; Review of organization-specific web site and specific reports, e.g. audits; sustainability reporting reports.
Social aspect	Freedom of association and collective bargaining
Aim and approach	The assessment aims to verify the compliance of the organization with freedom of association and collective bargaining standards. In particular 1) whether the workers are free to form and join association(s) of their choosing even when it could damage the economic interest of the organization, 2) whether the workers have the right to organise unions, to engage in collective bargaining, and to strike.
Suggested indicators	Employment is not conditioned by any restrictions on the right to collective bargaining Presence of unions within the organization is adequately supported (availability of facilities to union, posting of union notices, time to exercise the representation functions on paid work hours) Check the availability of collective bargaining agreement and meeting minutes (e.g. copies of collective bargaining negotiations and agreements are kept on file) Employee/union representatives are invited to contribute to planning of larger changes in the company, which will affect the working conditions Workers have access to a neutral, binding, and independent dispute resolution procedure
Generic data sources (examples)	International Trade Union Confederation Annual survey report ; UN Human Rights index on freedom of association; US Department of States country reports on human rights, including the Freedom of association and Collective bargaining

Specific data sources	Interview with directors or human resources officer; interview with workers and trade union representatives; NGO reports Verification of organizations' documents including sustainability reports; interview and/or questionnaire filled out by directors or human resources officer
Social aspect	Working time
Aim and approach	The assessment aims to verify if the number of hours effectively worked is in accordance with the ILO standards and when overtime occurs, compensation in terms of money or free time is planned and provided to the workers.
Suggested indicators	Number of hours effectively worked by employees (at each level of employment) Number of holidays effectively used by employees (at each level of employment) Respect of contractual agreements concerning overtime The organization provides flexibility
Generic data sources (examples)	International Trade Union Confederation, WTO country report • U.S. Department of State Human Rights Country Reports
Specific data sources	Interviews with workers, governmental agencies, management and NGOs • Review of audits • Review of time records Review of organization-specific reports, such as GRI reports or audits agreement or contracts between organizations and employees
Social aspect	Equal opportunities / discrimination
Aim and approach	The subcategory aims to assess equal opportunity management practices and the presence of discrimination in the opportunities offered to the workers by the organizations and in the working conditions.
Suggested indicators	Presence of formal policies on equal opportunities Announcements of open positions happen through national/regional newspapers, public job databases on the internet, employment services, or other publicly available media ensuring a broad announcement. Total numbers of incidents of discrimination and actions taken Composition of governance bodies and breakdown of employees per category according to gender, age group, minority, group membership, and other indicators of diversity Ratio of basic salary of men to women by employee category
Generic data sources (examples)	Division for the Advancement of Women – Department of Economic and Social affair • PSILCA (Discrimination) • SHDB (Gender Equity) • World Bank gender equality resources
Specific data sources	GRI Sustainability reports; Review of enterprise-specific reports; Review of violation records (can be national); Interview with NGOs; Interviews with human resources and management; sustainability reports
Social aspect	Community engagement
Aim and approach	This subcategory assesses whether an organization includes community stakeholders in relevant decision making processes. It also considers the extent to which the organization engages with the community, in general.
Suggested indicators	This subcategory assesses whether an organization includes community stakeholders in relevant decision making processes. It also considers the extent to which the organization engages with the community, in general. Diversity of community stakeholder groups that engage with the organization Number and quality of meetings with community stakeholders Organizational support (volunteer-hours or financial) for community initiatives
Generic data sources (examples)	U.S. Department of State annual country reports on human rights, including freedom of peaceful assembly and association and political participation • World Economic Forum annual country rankings on transparency of government policymaking and public trust of politicians
Specific data sources	Engage with the organization; Site visit or site-specific audit; Interviews with community members, employees, management, and NGOs; Review of organization-specific reports, such as sustainability reports or audits.
Social aspect	Local employment
Aim and approach	This subcategory assesses the role of an organization in directly or indirectly affecting local employment
Suggested indicators	Percentage of workforce hired locally Strength of policies on local hiring preferences Percentage of spending on locally-based suppliers
Generic data sources (examples)	Site visit or site-specific audit; Interviews with community members, employees, governmental agencies, management, and NGOs; Review of organization-specific reports, such as sustainability reports
Specific data sources	• ILO Key Indicators of the Labour Market for employment statistics by country and sector • PSILCA • World Economic Forum annual country rankings on networks, including local supplier quantity
Social aspect	Responsible communication
Aim and approach	The aim of the assessment is to evaluate the extent of responsible marketing that has been practiced by the organization, related to the product and services they produced.

Suggested indicators	The organization has a policy on responsible marketing The organization performs audit on the implementation of responsible marketing The organization receives monitoring and evaluation from the governing body on the implementation of responsible marketing The number of incidents of non-compliances with regulations and/or voluntary codes concerning product and service information/ marketing/ advertising and labeling, by incidents of non-compliance with regulations resulting in a fine or penalty; incidents of non-compliance with regulations resulting in a warning; and incidents of non-compliance with voluntary codes
Generic data sources (examples)	Commercial databases like Datamaran and MapleCroft; user protection agencies
Specific data sources	Interviews with management on regulations; Review of enterprise-specific reports, such as sustainability reports, SA8000 certifications, and annual reports

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