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Safe-and-Sustainable-by-Design (SSbD) as an enabler - Positioning SSbD within current chemistry frameworks

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ABSTRACT

Safe-and-Sustainable-by-Design (SSbD) aims to integrate functionality with safety and sustainability in an iterative and lifecycle thinking approach, starting already at the design stage of the innovation process. This proactive approach ensures that chemicals, materials, and other products are produced and used without being a threat to human and planetary health. In the authors' understanding, SSbD should ideally start with defining the function or service that is needed and how it can be delivered in the most sustainable way. This should include using the least amount of chemicals or even no chemicals when non-chemical or non-material alternatives are available (systems thinking). This perspective explores where SSbD fits into the bigger picture with respect to already existing chemistry frameworks such as Green Chemistry, Circular Chemistry, Chemistry within a Circular Economy, and Sustainable Chemistry. Analysing the design principles, assessment levels, and key aspects shows that SSbD is strongly interlinked with these chemistry concepts. Greener synthesis (Green Chemistry) and circular value chains (Circular Chemistry and Chemistry within a Circular Economy) are important aspects and objectives of SSbD, while the closed link and highest similarity is to Sustainable Chemistry as both operate on a system level and start with the function/service that needs to be provided. This in mind, the authors consider SSbD as an enabler of Sustainable Chemistry to accelerate the transition towards sustainability from the design stage, thereby moving the chemistry sector towards more sustainable practices, contributing to achieve the United Nations Sustainable Development Goals (SDGs), and ensuring humanity operates within the planetary boundaries.

1. Introduction

1.1. Need for new preventive approaches in innovation

Humanity currently faces a triple planetary crisis of climate change, biodiversity loss, and pollution that is destabilizing our Earth's systems (Carney Almroth et al., 2022). Major causes for these environmental crises are linked to anthropogenic chemicals. The chemical sector is energy- and resource-intensive and one of the major carbon dioxide emitters. Globally, chemical production has

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grown fifty-fold since 1950 and will triple again by 2050 in comparison to 2010, mainly outside Europe (EEA, 2017). The number of new chemicals being introduced to the market surpasses the rate at which hazard assessments can be conducted, resulting in a lack of sufficient safety information (including environmental hazards) associated with many chemicals (Kristiansson et al., 2021). As a result, adverse environmental effects are frequently detected even long after the chemical has already been put on the market (Johnson et al., 2020) and cleaning up is not possible at all or costly. The annual health related costs for PFAS alone were estimated 52–84 billion Euros in the European Economic Area (EEA) (Goldenman et al., 2019) and 60 billion US $ in the USA (Obsekov et al., 2023). Costs for environmental remediation are estimated up to 170 billion Euros for the EEA member countries and Switzerland (Goldenman et al., 2019). Whilst the average market price for PFAS is 19 €/kg, the social costs are estimated to be 18.700 €/kg (ChemSec, 2023; The Guardian, 2023).

Therefore, urgent action is needed to ensure in a precautionary approach (European Union n.d.; Holm et al., 2012) that chemical, material, product and process innovations are safe and sustainable. To move towards this goal, methodologies for the early-stage identification and rectification of emerging safety and sustainability issues (Peijnenburg et al., 2021) are needed such as the recently introduced Safe-and-Sustainable-by-Design (SSbD) approach (EC, 2020a; Caldeira et al., 2022; OECD, 2022; Cefic, 2021, 2022; Abbate et al., 2024).

The SSbD concept has been developed for achieving for instance climate neutrality, resource-efficiency, circular value chains, and the transition towards a toxic-free environment (EC, 2019, 2020a, 2020b, 2021). SSbD is an interdisciplinary approach aiming to integrate safety and sustainability considerations from the very beginning and throughout the entire innovation process in an iterative way; thereby ensuring that chemicals, materials, products, and processes do not pose a threat to human and planetary health from a lifecycle perspective. The SSbD concept as it is being brought to implementation considers the current available chemistry frameworks such as Green Chemistry, Circular Chemistry, and Sustainable Chemistry, yet an assessment on how SSbD relates to and supports these frameworks is missing.

1.2. Background on sustainability

Sustainability has become the major focus of policy ambitions and an ever-increasing societal demand in the last decades. Several working descriptions and definitions of *sustainability* exist (i.e. Brundtland, 1987; Laurett et al., 2021; Sala et al., 2013; Stupak et al., 2021) and have been recently combined by the OECD (2022). According to the OECD working description, *sustainability* supports *societal, economical, and environmental Sustainable Development Goals (SDGs) for our planet and for present and future generations. It refers to the use of the biosphere by present generations while maintaining its potential yield (benefit) for future generations. The safety concept for humans and the environment is transversal to all sustainability dimensions (environmental, social and economic)*. Sustainability has three main pillars, all of them overlapping and cross linked by safety: Planet/Biosphere/Environment, People/Society, and Prosperity/Economy. In short, *sustainability could be described as the ability of a material or chemical to provide products/services with desired functionalities without exceeding planetary boundaries, while ensuring wellbeing and other socio-economic benefits* (OECD, 2022).

Three different strategies are needed for achieving strong sustainability: *efficiency, sufficiency,* and *consistency* (Grunwald and Kopfmüller, 2006; Huber, 2000; Schäpke and Rauschmayer, 2014; EC, 2023). *Efficiency*, in general, aims to optimize the ratio of the desired output or benefit to the inputs used, such as resources (raw materials and energy), time or costs. In practical terms, efficiency is about achieving more with less; not only at the level of individual products, but also at the level of substance and material flows for societies and economies as a whole. This includes, for example, optimising the use of resources and minimising waste to reduce environmental impact and conserve resources. *Sufficiency*, on the other hand, calls for a change in lifestyles and consumption habits rather than in the way products are produced. It focuses on satisfying needs ('sufficient') rather than what is only wanted or 'nice to have'. In doing so, sufficiency challenges the dominant culture of high and over-consumption and instead promotes lifestyles that prioritise human and environmental well-being over material accumulation. Embracing sufficiency can include practices such as minimalism, sharing economies, alternative non-material business models, and mindful consumption patterns that reduce overall resource use, energy needs, pollution, and waste generation. *Consistency* in sustainability involves maintaining a balance between economic, social, and environmental factors over time, i.e. not thinking in isolated pillars and acknowledging that the planet is the basis of all, not economy. It involves implementing policies, strategies, and behaviours that are not only effective in the short term but also in the long run. This includes fostering resilience to environmental changes, preserving biodiversity, and promoting social equity to ensure that current actions do not compromise the ability of future generations to meet their needs (Brundtland, 1987).

Sustainability is strongly linked to the concept of the planetary boundaries that has been developed by Rockström et al. (2009) to define a safe operating space within which humanity can continue to develop and thrive. Exceeding these boundaries ("tipping points") can lead to unintended and potentially catastrophic consequences for the planet and human societies. A set of nine planetary boundaries has been defined, including climate change, ocean acidification, stratospheric ozone, biogeochemical nitrogen (N) cycle and phosphorus (P) cycles, global freshwater use, land system change, the rate of biodiversity loss, chemical pollution and atmospheric aerosol loading (Rockström et al., 2009). It has been recently shown that humanity is operating outside the safe space of seven out of the nine planetary boundaries (PB Science, 2025), including for novel chemical entities (Persson et al., 2022). While the concept creates an awareness that boundaries exist, there is the challenge of quantifying them to really know where the boundaries are. At the same time, there is a temptation to get as close to the boundaries as possible. This is why the precautionary principle is of high importance in this context.

From the policy side, one of the key documents is the 2030 Agenda for a Sustainable Development by the United Nations (UN) (UN, 2015). This agenda defines 17 SDGs, that provide a shared blueprint for peace and prosperity for people and the planet. The SDGs were developed aiming to end poverty and other human deprivations along with strategies that improve health and education, reduce

Table 1

Detailed overview of principles and keystones of Green Chemistry, Circular Chemistry, and Chemistry within a Circular Economy. As these principles are not fully comparable, the original order from the publications was kept. The text in blue are comments given by the authors.

Green Chemistry principles from the United States Environmental Protection Agency (EPA, 2024) based on Anastas and Warner (1998)	Circular Chemistry principles from Keijer et al. (2019)	Chemistry keystones for a circular economy from Kümmerer et al. (2020)
1. Prevent waste: Design chemical syntheses to prevent waste. Leave no waste to treat or clean up.	**1. Collect and use waste.** Waste is a valuable resource that should be transformed into marketable products.	**Keep molecular complexity to the minimum** required for the desired performance, including end of life (complex molecules require more synthesis steps, may have additional undesirable properties, and can be more difficult to recycle)
2. Maximize atom economy: Design syntheses so that the final product contains the maximum proportion of the starting materials. Waste few or no atoms. **This is a tool related to GC principle #1**	**2. Maximize atom circulation.** Circular processes should aim to maximize the utility of all atoms in existing molecules.	**Design products for recycling,** including all additives and other components of the product.
3. Design less hazardous chemical syntheses: Design syntheses to use and generate substances with little or no toxicity to either humans or the environment.	**3. Optimize resource efficiency.** Resource conservation should be targeted, promoting reuse and preserving finite feedstocks.	**Reduce and simplify diversity and dynamics** of substance, material, and product flows; e.g., use fewer chemicals overall (both number and quantity), design for less resource intensity, and adapt innovation speed of products to adaptation speed of recycling.
4. Design safer chemicals and products: Design chemical products that are fully effective yet have little or no toxicity. **This principle relates to GC principle #3**	**4. Strive for energy persistence**. Energy efficiency should be maximized.	**Avoid complex products** (e.g., multiple components, materials).
5. Use safer solvents and reaction conditions: Avoid using solvents, separation agents, or other auxiliary chemicals. If you must use these chemicals, use safer ones. **This principle relates to GC principle #3**	**5. Enhance process efficiency.** Innovations should continuously improve in- and post-process reuse and recycling, preferably on-site.	**Minimize use of product components** that cannot easily be separated and recycled (e.g., solvents, metals).
6. Increase energy efficiency: Run chemical reactions at room temperature and pressure whenever possible.	**6. No out-of-plant toxicity.** Chemical processes should not release any toxic compounds into the environment.	**Design products** not suitable for capture and recycling for complete fast mineralization at the end of their lives (e.g., pharmaceuticals, pesticides, personal care and cleaning products).
7. Use renewable feedstocks: Use starting materials (also known as feedstocks) that are renewable rather than depletable. The source of renewable feedstocks is often agricultural products or the wastes of other processes; depletable feedstocks are often fossil fuels (petroleum, natural gas, or coal) or mining operations.	**7. Target optimal design.** Design should be based on the highest end-of-life options, accounting for separation, purification and degradation.	**Prevent raw materials** from becoming critical through reduced use and efficient recovery and recycling (e.g., many metals).
8. Avoid chemical derivatives: Avoid using blocking or protecting groups or any temporary modifications if possible. Derivatives use additional reagents and generate waste. **This principle relates to GC principle #3.**	**8. Assess sustainability.** Environmental assessments (typified by the LCA) should become prevalent to identify inefficiencies in chemical processes.	**Avoid entropic losses and transfers** (e.g., dissipation of metals, energy).
9. Use catalysts, not stoichiometric reagents: Minimize waste by using catalytic reactions. Catalysts are effective in small amounts and can carry out a single reaction many times. They are preferable to stoichiometric reagents, which are used in excess and carry out a reaction only once. **This principles relates to GC principles #3 and #6.**	**9. Apply ladder of circularity.** The end- of-life options for a product should strive for the highest possibilities on the ladder of circularity.	**Avoid rebound effects** (e.g., using less carbon often means higher demand for metals). **This principle addresses regrettable substitution.**
10. Design chemicals and products to degrade after use: Design chemical products to break down to innocuous substances after use so that they do not accumulate in the environment.	**10. Sell service, not product.** Producers should employ service-based business models such as chemical leasing, promoting efficiency over production rate.	**Be responsible for/develop ownership of your product** throughout its complete life cycle, including recycling
11. Analyze in real time to prevent pollution: Include in-process, real-time monitoring and control during syntheses to minimize or eliminate the formation of byproducts.	**11. Reject lock-in**. Business and regulatory environment should be flexible to allow the implementation of innovations.	**Ensure traceability** and consider use of product digital passports (e.g., composition of products, components, and processes)
12. Minimize the potential for accidents: Design chemicals and their physical forms (solid, liquid, or gas) to minimize the potential for chemical accidents including explosions, fires, and releases to the environment.	**12. 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.	**Develop and apply circular metrics** (e.g., giving credit to the use of by-products).

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Table 1 (*continued*)

Green Chemistry principles from the United States Environmental Protection Agency (EPA, 2024) based on Anastas and Warner (1998)	Circular Chemistry principles from Keijer et al. (2019)	Chemistry keystones for a circular economy from Kümmerer et al. (2020)
		Change traditional chemical practices based on "bigger-faster" into "optimal adapted-better-safer" and change ownership to rent, lease, and share business models. **Keep processes as simple as possible** with a minimum number of steps, auxiliaries, energy, and unit operations (e.g., separations, purification). **Design processes for optimal material recovery** of auxiliaries, unused substrates, and unintended by-products (based on quality and quantity).

(gender) inequality, and support economic growth while tackling climate change and working to preserve the planet's oceans and forests (UN, 2015). For nearly all SDGs, at least the related sub targets, chemistry plays a role.

1.3. Aim of this study

This perspective aims to explore the links between SSbD and the frameworks of *Green Chemistry*, *Circular Chemistry*, *Chemistry within a Circular Economy* and *Sustainable Chemistry*. These established chemistry frameworks are already being applied in practice, moving the chemical sector towards greener or more environmentally friendly chemicals and production processes, and some even beyond, including also social and economic sustainability aspects. By analysing these concepts and identifying their limitations, this study seeks to identify the unique role that SSbD can achieve in accelerating the transition of the chemical industry towards more sustainability.

2. Methods

A literature review was performed to identify descriptions on the concepts of *Green Chemistry*, *Circular Chemistry*, *Chemistry within a Circular Economy*, *Sustainable Chemistry*, and SSbD as well as comparison studies between these concepts. Literature sources were open databases: scientific publications, policy documents and papers as well as public reports. Core keyword groups: "green chemistry" OR "benign by design"; "sustainable chemistry" OR "sustainability in chemistry"; "circular chemistry" OR "chemistry for a circular economy"; SSbD OR "safe-and-sustainable-by-design"; above terms AND policy OR guidance OR framework OR definition OR criteria OR key characteristics; Combination of terms: comparison, definition, framework, implementation, guidance, review [("sustainable chemistry" OR "green chemistry") AND (definition OR framework OR criteria); ("Safe and Sustainable by Design" OR SSbD) AND (guidance OR policy OR framework)].

For the scientific literature (peer-reviewed and scholarly) sources included: Web of Science (multidisciplinary citation indexing for high-impact journals); Scopus (broad coverage of journals, conference proceedings, and reviews); PubMed/MEDLINE (for health-related chemistry intersections and toxicology); Google Scholar (supplementary broad search to capture grey literature and citations); and ScienceDirect (Elsevier).

For the policy reports, and grey literature sources included: OECD Library (OECD reports and monographs (e.g., Sustainable Chemistry series); European Union Publications/Publications Office (EU frameworks and official guidance (e.g., European Environment Agency (EEA), EC reports); National environment agencies and ministries (examples: German Environment Agency (UBA); Industry associations and consortia (Cefic, GC3 (Green Chemistry & Commerce Council), ISC3); NGOs and advocacy groups (ChemSec and similar organizations that publish SSbD or chemical policy guidance); Institutional repositories and think tanks such as university policy centers, and research institutes.

Inclusion criteria included: i) documents that explicitly address one or more of the target concepts: green chemistry, circular chemistry, sustainable chemistry, chemistry for a circular economy, and SSbD; ii) primary focus on contemporary literature (e.g., last 15 years) but include seminal works regardless of date (e.g., Anastas and Warner, 1998); specifying exact cut-off (e.g., up to 2024).

Exclusion criteria included: i) documents that mention keywords only tangentially without substantive conceptual, methodological, or policy content on the target concepts; ii) Narrow technical reports without conceptual relevance: highly specialized experimental reports that do not address conceptual definitions, frameworks, or policy implications of the target concepts.

The results from the literature review are shown in Table S1 of the Supplementary Material.

The literature review results were then analysed by experts in Sustainable Chemistry and SSbD to identify the boundaries and limitations of each and identify the unique role of SSbD in relation to these concepts.

Table 2
Criteria, rules, and key characteristics of Sustainable Chemistry defined by different organizations (aligned to the Key Characteristics of Sustainable Chemistry (Kümmerer et al., 2021).

Key characteristics of Sustainable Chemistry from ISC3 (Kümmerer et al., 2021)	Sustainable Chemistry criteria categories from ECOSChem (2023)	General Principles (GP) of Sustainable Chemistry from UBA (2009) [a]	Golden Rules (GR) of Sustainable Chemistry from UBA (2016) [a]
1. Holistic: Guiding the chemical science and the chemical sector towards contributing to Sustainability in agreement with sustainability principles and general understanding and appreciating potential interdependencies including long-distance interactions and temporal gaps between the chemical and other sectors.	**Climate and Ecosystem impacts**[b]: • Utilization of renewable, non-toxic chemical building blocks • Avoidance of negative impacts on natural resources, the climate, and biodiversity • Minimization of energy use and greenhouse gas emissions	**GP2 - Quantitative development**[b]: Reduction of the consumption of natural resources, which should be renewable wherever possible, avoidance or minimization of emission or introduction of chemicals or pollutants into the environment. Such measures will help to save costs.	
2. Precautionary: Avoiding transfer of problems and costs into other domains, spheres and regions at the outset, preventing future legacies and taking care of the legacies of the past including linked responsibilities.	**Health and Safety Impacts** • Absence of hazards to people or ecosystems • Prevention of environmental releases that persist or bioaccumulate	**GP4 - Action instead of reaction:** 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.	**GR1:** 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.
3. Systems thinking: Securing its interdisciplinary, multidisciplinary and transdisciplinary character including a strong disciplinary basis but taking into account other fields to meet Sustainability to its full extent. Application as for industrial practice including strategic and business planning, education, risk assessment and others including the social and economical spheres by all stakeholders.			
4. Ethical and social responsibility: Adhering to value to all inhabitants of plant earth, the human rights, and welfare of all live, justice, the interest of vulnerable groups and promoting fair, inclusive, critical, and emancipatory approaches in all its fields including education, science, and technology.	**Equity and Justice:** • Authentic engagement of potentially impacted communities • Protection of workers, marginalized communities, and vulnerable groups • Prioritization of innovations that remediate past harms • Strengthening of local economies and product access and affordability		**GR8:** 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. **GR9**[b]**:** Furthermore, products should not be put on the market for which a societal benefit and a benefit for consumers can not be identified.
5. Collaboration and Transparency: Fostering exchange, collaboration, and right to know of all stakeholders for improving the sustainability of business models, services, processes and products and linked decisions including ecological, social, and economic development on all levels. Avoiding all "green washing" and "sustainability washing" by full transparency in all scientific and business activities towards all stakeholders, and civil society.	**Transparency:** • Disclosure and accessibility of health, safety, and environmental data • Open access and verification of sustainability claims • Availability of chain-of-custody information for chemicals and materials		
6. Sustainable and Responsible Innovation: Transforming fully the chemical and allied industries from the		**GP5 - Economic innovation**[b]: Sustainable chemicals, products and production methods produce	

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Table 2 (*continued*)

Key characteristics of Sustainable Chemistry from ISC3 (Kümmerer et al., 2021)	Sustainable Chemistry criteria categories from ECOSChem (2023)	General Principles (GP) of Sustainable Chemistry from UBA (2009) [a]	Golden Rules (GR) of Sustainable Chemistry from UBA (2016) [a]
molecular to the macroscopic levels of products, processes, functions and services in a proactive perspective towards sustainability including continuous trustworthy, transparent and traceable monitoring.		confidence in industrial users, private consumers and customers from the public sector and thus, result in competitive advantages.	
7. Sound Chemicals Management: Supporting the sound management of chemicals and waste throughout their whole life cycle avoiding toxicity, persistency and bio-accumulation and other harm of chemical substances, materials, processes, products and services to humans and the environment.			**GR4:** Do not 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[c] approach.
8. Circularity: Accounting for the opportunities and limitations of a circular economy including reducing total substance flows, material flows, product flows, and connected energy flows at all spatial and temporal scales and dimensions especially with respect to volume and complexity.	**Circularity** • Design of products with an appropriate lifetime • Enablement of safe reuse and recycling • Emphasis on resource efficiency and waste prevention		**GR5**[b]**:** 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.
9. Green Chemistry: Meeting under sustainable chemistry application as many as possible of the 12 principles of green chemistry with hazard reduction at its core when chemicals are needed to deliver a service or function whenever and wherever this complies with sustainability.		**GP1 - Qualitative development:** 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	**GR3:** 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, do not bioaccumulate and do not widely disperse in the environment! With these substances you have to put less effort in risk management measures. **GR7:** 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.
10. Life Cycle: Application of the above-mentioned key characteristics for the whole lifecycle of products, processes, functions and services on all levels, e.g. from molecular to the macroscopic levels and all sectors in a pro-active perspective towards sustainability.		**GP3 - Comprehensive life cycle assessment:** Analysis of raw material production, manufacture, processing, use and disposal of chemicals and discarded products in order to reduce the consumption of resources and energy and to avoid the use of dangerous substances	**GR2:** Using problematic substances assess the different uses **and** potential users of the substance as such. If the substance cannot be exchanged you have to take responsibility for the consequences of its use. Never only evaluate the substance in isolation but think through the entire lifecycle! **GR6**[b]**:** 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.

[a] considered in the SSbD framework development.
[b] partly.
[c] COSHH: Control of substances hazardous to health.

3. Results and discussion

3.1. Current chemistry frameworks

3.1.1. Green, circular, and sustainable chemistry

Green Chemistry aims for pollution prevention. Already in the 1970s and 1980s pollution prevention was practiced and commercialized in the chemical industry supported by some academics (Clark et al., 1989; Kletz, 1978; Murphy, 2018, 2021; Poliakoff and Kletz, 2013; Royston, 1979; Sheldon, 1992, 2017; Trost, 1991; Tundo and Aricó, 2007; UN, 1978). The term *Green Chemistry* was introduced in the early 1990s by the U.S. EPA and followed by a definition of twelve *Green Chemistry* principles in 1998 (Anastas and Warner, 1998). These principles guide chemists on the design and synthesis of less toxic and more environmental-friendly chemical products and processes generating less waste and using less energy. The twelve principles address important aspects to reduce impacts on human and environmental health such as preventing waste and pollution, using less hazardous chemicals, using less energy, and use of renewable feedstocks (Table 1). While *Green Chemistry* does not address the aspect of circularity itself, it can be seen as a tool to contribute to the transition to circularity and to the circular economy (Chen et al., 2020; Linder, 2017; Loste et al., 2020).

Circular Chemistry is focused on enabling the transition of chemistry to a circular economy (Keijer et al., 2019). The concept is also based on twelve principles (Table 1) in analogy to *Green Chemistry;* keeping six of the original principles and substituting six to address aspects of a circular economy (i.e. applying the ladder of circularity), an environmental sustainability assessment, as well as policy aspects and service-based business models (Keijer et al., 2019). With this, *Circular Chemistry* is a more holistic approach compared to *Green Chemistry* and underlines the interconnectivity between chemistry, economy, policy, and environmental science (Mutlu and Barner, 2022). However, for achieving strong sustainability, there are some missing aspects and limitations (Korhonen et al., 2018; Giampietro, 2023; De Man, 2023) which are discussed in Chapter 3.1.2.

The closely related concept ***Chemistry within a Circular Economy*** (Kümmerer et al., 2020) also addresses the role of chemistry within a circular economy. The authors identified fifteen chemistry keystones for the circular economy that highlight the need for simplifying complexity of products and product flows (Table 1). Chemical products should be designed as simple in composition as possible, with a minimized use of additives and without toxic compounds that are not easily separated for recovery. Furthermore, product flows should be kept as separate as possible at all life cycle stages to avoid mixing of varying constituents.

Sustainable Chemistry provides guiding principles and a broader systems thinking approach for achieving sustainability (Böschen et al., 2003; Hutzinger, 1999; Krasnodębski, 2023). *Sustainable Chemistry* as described by several authors (Blum et al., 2017; Kümmerer, 2017; Kümmerer et al., 2021) goes beyond the afore mentioned *Green Chemistry* and *Circular Chemistry* concepts following the guiding question: how to produce better and more from less? (Marion et al., 2017). *Sustainable Chemistry* is less product-centred and more service/function-oriented (Elschami and Kümmerer, 2018) and includes sufficiency considerations such as alternative non-chemical approaches to deliver a desired function or service by omitting chemicals or chemical products completely. Other aspects such as the increase of market opportunities and application of corporate social responsibility are also considered part of *Sustainable Chemistry* (Blum et al., 2017). Several organizations have defined criteria, roles, or key characteristics for *Sustainable Chemistry* (Table 2). ECOSChem (ECOSChem, 2023; Cannon et al., 2023) adopted some of the key characteristics previously defined by the International Sustainable Chemistry Collaborative Center (ISC3) (Kümmerer et al., 2021) and lists for example transparency and justice as *Sustainable Chemistry* criteria. However, their understanding of *Sustainable Chemistry* is still very much product-focussed, neglecting sufficiency. Therefore, it is very close to *Green Chemistry* as they define it as *the development and application of chemicals, chemical processes, and products that benefit current and future generations without harmful impacts to humans or ecosystems* (ECOSChem, 2023; Cannon et al., 2023).

The authors want to stress that caution is needed in the interchangeable use of the terms ‘green’, ‘circular’, and ‘sustainable’. Making a chemical 'greener' (following the principles of *Green Chemistry*) does not necessarily mean that it is more circular or even more sustainable (Keijer et al., 2019; Kümmerer, 2017; Kümmerer et al., 2021). Similarly, making a material, chemical, or chemical product circular does not necessarily mean that it is greener or even more sustainable - this needs to be carefully assessed on a case-by-case basis. "Green", "circular" and "sustainable" are all individual human values that overlap to a large extent but cannot be seen as synonyms (Fig. 4).

3.1.2. Sustainable chemistry as a holistic framework for achieving sustainability

Comparing the chemistry frameworks described in Chapter 3.1.1, *Sustainable Chemistry* is the only framework encompassing efficiency, sufficiency, and consistency strategies to reach sustainability. *Sustainable Chemistry* is a holistic framework giving guidance on how chemistry as a scientific and economic asset spanning multiple supply chains and consequently the whole life cycle, not just the value chain, can comply with all sustainability dimensions (environmental, social, economic) for the preservation of our planet. Therefore, *Sustainable Chemistry* is the understanding and practice of chemistry which is closest to sustainability whereas *Circular Chemistry* and even less *Green Chemistry* do not have this strong sustainability perspective. *Sustainable Chemistry* strives first for service and function without the need of chemical products (e.g., by wise construction of roofs which results in ‘no need’ for chemicals such as biocides to protect the building's façade, or by offering fruits or vegetables package-free). If such are needed, however, they should be designed for both, circulation and recycling and only then synthesized according to the principles of Green Chemistry (Table 1). Products which cannot be recycled should be avoided (Kümmerer et al., 2021) and the ones that enter into the environment should be designed for fast and full mineralization in the environment at the end of their life, e.g., by applying the Benign by Design concept (Boethling et al., 2007; Kümmerer, 2007, 2010). Chemicals that can be circulated, especially within business to business (B2B) and cannot reach the environment have to be designed for stability instead.

While the concepts of *Green Chemistry* and *Circular Chemistry* and their principles (Table 1) are both important for chemistry to contribute to sustainability, they do not address all sustainability aspects as covered by *Sustainable Chemistry*. Some of these missing sustainability aspects include i) systems thinking, ii) thermodynamics in circularity and recycling strategies iii) addressing the complexity of products and materials flows in modern industrial societies iv) trade-off considerations (i.e. development of renewable or bio-based products at the cost of deforestation or of farmland and food production), and v) the consideration of social and economic sustainability aspects, and vi) sufficiency. These aspects are further discussed below in more detail.

3.1.2.1. Systems thinking is needed. Systems thinking looks at a system as a whole, not just as a collection of parts, and also focuses on the system behaviour changes over time (Orgill et al., 2019; Mahaffy and Elgersma, 2022). Systems thinking, rather than individual and disconnected foci, is needed to ensure that chemistry successfully contributes to sustainability in the long term. The total substance and material flows need to be addressed and we, as a society, have to overcome the assumption that if we keep things in circulation and recycle them, there are no limits anymore.

Other aspects that are considered in systems thinking are the unwanted side-effects and possible rebound effects, e.g., through the reduction of waste. For example, different recycling routes for complex consumer products such as electronics and batteries can result in very different recovery rates for specific valuable metals. During recycling, a loss of materials is expected. Recycling of complex products is often a trade-off between bulk and minor element recycling, where often the one material will (in more or lesser extent) be "sacrificed" for the recovery of the other. The overall recycling efficiency also depends on the design of the products, the collection and sorting logistics, and the energy consumption (Reuter et al., 2018).

Systems thinking also considers the issue of chemicals, materials, and products that cannot be collected at their end of life. Many products cannot be collected and recycled because they are dispersed into the environment due to their open application (such as pesticides, personal care products, laundry detergents, abrasions from surfaces). Therefore, these products have to be designed for degradation keeping their end-of life fate and respective environmental conditions in mind.

3.1.2.2. Limitations of recycling due to thermodynamics. The *Circular Chemistry* concept advocates for a waste-free chemical industry (Keijer et al., 2019), which is in contrast with the basic laws of thermodynamics. Both a zero-waste industry and zero-waste circular economy are impossibilities due to thermodynamics (De Man, 2023). Based on *Circular Chemistry* principles (Table 1) the input of materials and their consumption, in particular virgin materials, is minimized. However, to come up with the same grade, properties and quality of recycled materials (e.g., metals and plastics) virgin material and energy has to be always added. Because products are often not designed for circularity, each recycling loop often decreases the quality of the material excluding the new products from several former applications. This often results in a single cycle and thus making "endless" recycling not possible. There is always a loss and downgrading of part of the material during use, collection and recycling. This is just one example of a general principle "there is no up-cycling, only downcycling" from a material and natural science (thermodynamics) point of view. The term upcycling commonly refers to recycling of waste or products at the end of their life, i.e., turning waste or used products of low economic value into products of higher economic value. However, there can only be an economic re-valorization of a portion of a waste material.

3.1.2.3. The diversity and complexity of products and product flows are a hindrance for circularity. The *Green Chemistry* principles focus on the individual molecule and do not address the issue of complex products, such as mixtures at the atomic, molecular and building block level, which hinders circularity options at the end of the product's life. In addition, the consideration of total substance and materials flows beyond the synthesis of individual chemicals is lacking. As it was previously put '*complexity is the enemy of circularity*' (Clark, 2022; Kümmerer et al., 2020), and therefore product composition and materials flows should be kept as simple and separate as possible to not hinder collection, sorting and dismantling processes at the product's end of life. However, a certain functionality is required by the application and needs to be preserved, therefore a certain composition and degree of complexity is always required. The challenge is to find the optimum of this compromise. For example, polyethylene is a basic constituent of many plastic materials which differ in compositions (e.g., caused by additives, degree of polymerisation i.e. chain length and average molecular weight) and grades, needed for functionality of different products (e.g. high density, low density, linear low density, ultra-high molecular weight, crosslinked). Here, product design balancing functionality with complexity is of great importance; bringing recyclability-by-design to chemicals and products that are in principle suitable for a circular economy (Kümmerer et al., 2020). Product design is needed on how products best fit in an efficient infrastructure to optimize closed loops or have open loops for secondary use in another application. This needs to be combined with the design for recycling (starting with ease of disassembly and then separability) to avoid the use of chemicals or products that are challenging to recycle. These issues need to be resolved if we, as a society, intend to fulfil the circular economy ambition and goal as far as possible.

3.1.2.4. Trade-off considerations. The *Green Chemistry* Principle 7 (Table 1) calls for the use of renewable rather than depletable feedstocks. However, it is important to note that there are many challenges associated with using 'renewable'[1] or 'bio-based'[2] resources that do not always make them 'greener' or even more sustainable. For example, renewable resources require additional land, water as well as fertilisers and pesticides, the latter of which may lead to environmental pollution and risks to human health. Often, additional resources are needed for harvesting and processing, resulting in more waste. One example are ionic liquids for cellulose extraction from wood (Swatloski et al., 2002; Szabó et al., 2023), which also need to be synthesized and may be toxic and persistent in the environment (Amde et al., 2015). When using renewable/bio-based chemicals or materials there is the risk that the resources are not sourced in a sustainable manner and the land used competes with food production or comes from deforestation. This is often not transparently assessed or communicated. For this to change, regenerative practices (Fischer et al., 2024) have to be organised, such as sustainable/regenerative farming, in such a way that farmers can earn a living from it, and to create also social benefits. While *Circular*

[1] Renewable resource - resource that is grown, naturally replenished or cleansed on a human time scale [SOURCE: ISO 21930:2017, 3.6.2].

[2] Bio-based - derived from biomass [SOURCE: EN 17228:2019, 3.1]. Bio-based polymer - polymer wholly or partly derived from biomass [SOURCE: EN 17228:2019, 3.2].

Table 3
Definitions and working descriptions of SSbD.

Organisation	Year	Definition/Working Description	Reference
EC	2020	*'At this stage, safe and sustainable-by-design can be defined as 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* ***lifecycle perspective****.'*	EC (2020a)
Cefic	2021	*'The chemical industry defines Safe and Sustainable-by-Design as a* ***process to innovate*** *and put on the market chemicals, materials, products* ***and technologies*** *that are safe and deliver environmental, societal, and/or economical value through their applications. Those chemicals, materials, products and technologies enable accelerating the transition towards* ***a circular economy*** *and climate-neutral society and preventing harm to human health and the environment throughout the* ***life cycle****.'*	Cefic (2021)
JRC	*2022*	*'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)*)'*	Caldeira et al. (2022)
OECD	2022	*'Safe and sustainable by design (SSbD) can be described as an approach that focuses on providing a* ***function (or service)****, while avoiding onerous environmental footprints and chemical properties that may be harmful to human health or the environment.* *In essence, the SSbD approach aims to identifying and minimising, at an* ***early phase of the innovation process****, the impacts concerning safety for humans and the environment and for sustainability, minimising the environmental footprint, in particular regarding climate change and resource use and, protecting ecosystems and biodiversity, taking a lifecycle perspective. The SSbD approach addresses the safety and sustainability of the material/chemical/product and associated processes along the whole* ***life cycle****, including all the* ***steps of the research and development (R&D) phase****, production, use,* ***recycling and disposal****.'*	OECD (2022)
Cefic	2022	*'Cefic and its members have defined Safe and Sustainable-by-Design (SSbD) as an* ***iterative process*** *guiding* ***innovation*** *and the placement on the market of chemicals, materials, products, processes* ***and services*** *that are safe, and deliver environmental, societal, and/or economical value through their applications. In scope are new chemicals, materials, products, processes and services, as well as* ***re-designing*** *existing ones.'*	Cefic (2022)

Chemistry acknowledges that resource renewability alone is not a measure of sustainability (Keijer et al., 2019), the major issue identified is the (often lacking) material circulation ('what is the difference between an oil-based or bio-based plastic soup in our oceans?' (Keijer et al., 2019)).

The use of these drop-in materials can also lead to 'lock-ins' with established systems doing 'business as usual' instead of adopting new approaches, e.g. moving to service-based business models or developing or adapting new technologies and infrastructure that support circular processes. Therefore, despite the benefits of drop-in materials, there is also a downside. Such drop-in approaches may only be an interim solution, i.e. a technology that contributes to the transformation but is not the final and desired outcome of the required transformation. This issue will always arise and demonstrates the importance of systems thinking (and carefully defining system boundaries) and avoiding addressing one sustainability issue without recognising negative impacts on others, particularly those that are offset in time and space.

3.1.2.5. Consideration of social and economic sustainability aspects. Sustainability consists of environmental, social, and economic dimensions. All these three dimensions of sustainability are interconnected, not isolated pillars. Social sustainability focuses on people and their well-being; enforcing the confirmation of basic necessities of people and this includes issues such as fair labour practices, no gender bias, no sexual harassment, quality education, equal opportunities, community development, no child labour, work-life balance, health and safety, protection, human rights and wellness (UNEP, 2009). This is also being practised through Corporate Social Responsibility (CSR). The economic dimension of sustainability supported by life cycle costing (LCC) allows justifying environmentally and/or socially responsible strategies that require a high investment but would provide the best value for money across the life cycle. Assessing social and economic dimensions of sustainability, in addition to the environmental dimension, in a mid-term and long-term systems thinking approach is vital for sustainability, yet neither social nor economic sustainability aspects are addressed within the principles of *Green* and *Circular Chemistry* (Table 1).

3.1.2.6. Sufficiency needs to be addressed. Sufficiency is not only "doing better with less" but producing more of those things that increase the social foundation and people's wellbeing, rather than producing marketable goods more efficiently (Kallis et al., 2025; Kromand et al., 2025; Jungell-Michelsson and Heikkurinen, 2022; André, 2024). Sufficiency is a mindset that prioritises human and environmental well-being over material accumulation and includes practices such as minimalism, sharing economies, alternative non-material business models, and mindful consumption patterns that reduce overall resource use, energy needs, pollution, and waste generation.

Sufficiency is not addressed in *Green Chemistry* and only marginally addressed in *Circular Chemistry* (through principle 10, the promotion of service-based business models). A strong sustainability impact can be achieved only by embracing sufficiency, consistency, and efficiency all together. André (2024) proposes a sufficiency LCA where product alternatives need to be similar enough so

Fig. 1. Prioritization of actions considering the zero-pollution hierarchy which favours a preventive approach instead of a mitigation approach (adapted from EC, 2021).

that the 'what' component of the functional unit can be equal, while the other components, 'how much', 'how long', and 'how well', are allowed to be non-equal. The proposed sufficiency LCA allows for functional non-equivalence of compared product alternatives, which is not allowed or neglected in conventional LCAs. Further research is needed to ensure sufficiency is included in chemistry frameworks.

3.2. Safe and sustainable-by-design (SSbD)

3.2.1. What is SSbD?

Safe and Sustainable-by-Design was first defined by the European Commission (EC) as '*a pre-market* [voluntary, iterative and holistic] *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 lifecycle perspective'* in 2020 (EC, 2020a). Since then, also other institutions published definitions and working descriptions on SSbD (Table 3), that differ slightly in scope (i.e. only chemicals or also including materials and products) but show a high consensus in general (Apel et al., 2024).

In the authors' understanding, SSbD should be expanded from the working descriptions shown in Table 3. It should start with defining the function or service that is needed and how it can be delivered in the most sustainable way, including using the least amount of chemicals or no chemicals at all when non-chemical or non-material alternatives are available. With this in mind, SSbD is more then only a design approach for chemical and materials but starts with the big picture in mind and can support moving *Sustainable Chemistry* forward. If a chemical or chemical products in required, SSbD aims to integrate this desired functionality with safety and sustainability considerations in an iterative, systems and lifecycle thinking approach starting already at the design stage of the chemical, material, or product development and thereby ensuring that these are produced and used without contributing to exceeding acceptable ecological limits, e.g., the planetary boundaries. SSbD is not focused only on chemical-by-chemical substitution but rather goes beyond by identifying the biggest safety and sustainability challenges along the life cycle and steering SSbD strategies towards optimization of impact and purpose driven innovation. SSbD helps to locate the safety and sustainability impact on a map and relocate the SSbD strategies for maximum impact in this multidimension space of safety and sustainability (Fig. 1). With this understanding, SSbD shows a close relation to *Sustainable Chemistry* as both concepts operate on a system level and start with the function/service that needs to be provided. Only by applying all three sustainability strategies (efficiency, consistency, and sufficiency), a strong sustainability impact can be achieved.

In 2022, a framework for the definition of criteria and evaluation procedure for chemicals and materials was published by the EC's Joint Research Centre (JRC) (Caldeira et al., 2022), followed by a Methodological Guidance (Abbate et al., 2024) and a revised SSbD framework (Garmendia Aguirre et al., 2025). The revised SSbD framework proposed a holistic, iterative and tiered approach to apply SSbD in research and Innovation (R&I), consisting of SSbD framework principles, a scoping analysis, a safety and sustainability assessment, evaluation and documentation. The SSbD framework principles include i) Assessments consider the entire SSbD system including chemicals/materials, processes and products under study and their related life cycles; ii) The SSbD concept builds on multidisciplinary engagement of the life cycle actors and company experts to ensure that both safety and sustainability are considered throughout the entire innovation; iii) Safety and sustainability aspects are addressed with a holistic perspective throughout the innovation. The iterative approach in innovation also takes into consideration the inherent uncertainties and trade-offs in each iteration. SSbD is not static, but evolves over time, in function of new information on hazards and uses, new challenges and needs and new available innovative solutions. The tiered approach implies the gradual reduction of uncertainties by identifying information needs

Table 4
SSbD design guiding principles and assessments steps of the revised JRC SSbD framework (Garmendia Aguirre et al., 2025).

SSbD Design Guiding Principles	Assessments Steps of the Safety and Sustainability Assessment
SSbD1 Material efficiency 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. (based on GC2, CC2, GC8, GC9, GC5, CC5, GC1, GP2[a])	**Hazard Assessment** The assessment focuses on the hazard properties (human health, environmental and physical hazards) of the manufactured chemicals and materials.
SSbD2 Minimize the use of hazardous chemicals/materials Preserve functionality of products while reducing or completely avoid using hazardous chemicals/materials where possible. (based on GC3, GP1, GR1, GC4, GE1, GR3, GC5)	**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).
SSbD3 Design for energy efficiency Minimize the overall energy used to produce a chemical/material in the manufacturing process and/or along the supply chain. (based on GC6, CC4, GE4, GE5, CC8, GE8, GE10, GE3, GR7, GC8, GC9, CC10)	**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.
SSbD4 Use renewable sources Target resource conservation, either via resource closed loops or using renewable material/secondary material and energy sources. (based on GC7, CC3, GE12, GP2)	**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.
SSbD5 Prevent and avoid hazardous emissions Apply technologies to minimize and/or to avoid hazardous emissions or pollutants in the environment. (based on GE11, GC11, CC6, GP2)	**Social Sustainability, Economic Sustainability** This step is at an exploratory phase. It presents 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.
SSbD6 Reduce exposure to hazardous substances 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. (based on GC12, GR4, GP1)	
SSbD7 Design for end-of- life 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. (based on GC10, CC1, CC7, GE11, CC9, GE9, GE6, GE7)	
SSbD8 Consider the whole life cycle Apply the other design principles thinking through the entire life cycle, from supply-chain of raw materials to end-of-life in the final products. (based on GE6, GR2, GP3, GR6, GR8)	
SSbD9 Ensure responsible sourcing and minimise social risks Avoid that procurements are linked with severe human rights and labour rights abuses, as well as other unethical practices. Perform a suppliers' assessment based on social performance and risk. Include Environmental, Social and Governance (ESG) performance as a criterion for suppliers' selection. Scrutinise suppliers operating in conflict-affected and high-risk areas. (based on GR8)[b]	

[a] Green Chemistry Principle (Anastas and Warner, 1998, Table 1), GE: Green Engineering Principle (Anastas and Zimmerman, 2003), CC: Circularity Chemistry Principle (Keijer et al., 2019, Table 1), GP: General Principles of Sustainability Chemistry (UBA, 2009, Table 2), GR: UBA Golden Rule (UBA, 2016, Table 2).
[b] Based on author's analysis.

and gathering or generating data for each iteration, as the innovation process progresses; and iv) The SSbD concept implies transparency of the assessment and traceability of the fulfilment of the principles throughout the entire innovation (Garmendia Aguirre et al., 2025). In addition, the SSbD design principles (Table 4) guiding the design of SSbD chemicals, materials, and products have strong links to the principles of *Green Chemistry* (from Anastas and Warner, 1998, Table 1), *Green Engineering* (from Anastas and Zimmerman, 2003), *Circular Chemistry* (from Keijer et al., 2019, Table 1) and *Sustainable Chemistry* (from UBA, 2009, 2016, Table 2); highlighting the interconnectivity between these concepts. The aspect of *efficiency* is strongly linked in these design principles (i.e. material and energy efficiency).

The safety and sustainability assessment verifies whether a design meets SSbD criteria by combining hazard, exposure, functionality, and sustainability evidence across the product life cycle. It is explicitly iterative as the assessment outputs continuously inform design or go/no-go decisions in the design phase. The core components of the assessments are i) Initial screening and problem framing performs rapid checks for obvious hazards, regulatory status, and data gaps to set assessment boundaries; ii) Safety assessment

SSbD Framework and Design Principles
- Assessments consider the entire SSbD system
- The SSbD concept builds on multidisciplinary engagement of the life cycle actors and company experts
- Safety and sustainability aspects are addressed with a holistic perspective throughout the innovation.
- The SSbD concept implies transparency of the assessment and traceability of the fulfilment of the principles throughout the entire innovation
- **SSbD1** Material efficiency
- **SSbD2** Minimise the use of hazardous chemicals/materials
- **SSbD3** Design for energy efficiency
- **SSbD4** Use renewable sources
- **SSbD5** Prevent and avoid hazardous emissions
- **SSbD6** Reduce exposure to hazardous substances
- **SSbD7** Design for end-of- life
- **SSbD8** Consider the whole life cycle
- **SSbD9** Ensure responsible sourcing and minimise social risks

Green Chemistry Principles
1. Prevent waste
2. Maximize atom economy
3. Design less hazardous chemical syntheses
4. Design safer chemicals and products
5. Use safer solvents and reaction conditions
6. Increase energy efficiency
7. Use renewable feedstocks
8. Avoid chemical derivatives
9. Use catalysts, not stoichiometric reagents
10. Design chemicals and products to degrade after use
11. Analyze in real time to prevent pollution
12. Minimize the potential for accidents

Circular Chemistry Principles
1. Collect and use waste
2. Maximize atom circulation
3. Optimize resource efficiency.
4. Strive for energy persistence
5. Enhance process efficiency
6. No out-of-plant toxicity
7. Target optimal design
8. Assess sustainability
9. Apply ladder of circularity
10. Sell service, not product
11. Reject lock-in
12. Unify industry and provide coherent policy framework

Chemistry keystones for a circular economy
- Keep molecular complexity to the minimum
- Design products for recycling
- Reduce and simplify diversity and dynamics
- Avoid complex products
- Minimize use of product components
- Design products not suitable for capture and recycling for complete fast mineralization at the end of their lives
- Prevent raw materials from becoming critical through reduced use and efficient recovery and recycling
- Avoid entropic losses and transfers
- Avoid rebound effects
- Be responsible for/develop ownership of your product
- Ensure traceability
- Develop and apply circular metrics
- Change traditional chemical practices
- Keep processes as simple as possible
- Design processes for optimal material recovery

Fig. 2. Graphical visualisation of Table 1 complemented by the SSbD framework and design principles as proposed by Garmendia Aguirre et al. (2025). As these principles are not fully comparable, the original order from the publications was kept (Green Chemistry principles from the United States Environmental Protection Agency (EPA, 2024) based on Anastas and Warner (1998); Circular Chemistry principles from Keijer et al. (2019); Chemistry keystones for a circular economy from Kümmerer et al. (2020)).

includes the evaluation of intrinsic toxicological and ecotoxicological properties using existing data, read-across, and in vitro/in silico methods where appropriate and considering estimation of potential human and environmental exposures across manufacture, use, and end-of-life; iii) Life-cycle assessment (LCA) often using simplified LCA or scenario modelling in early tiers. Sustainability indicators include the assessment of climate, resource use, circularity potential, and socio-economic aspects using selected indicators and metrics; iv) Functionality and performance verification includes the demonstration that the substance or material achieves the intended technical function without unacceptable trade-offs. Each of these components is applied with increasing depth as the innovation progresses from concept to market, conserving resources while reducing uncertainty (Garmendia Aguirre et al., 2025).To ensure that the impacts of chemicals, materials, and products and its production system(s) are within the planetary boundaries, an absolute sustainability assessment is required. While this absolute sustainability assessment is mentioned as the ultimate goal of the SSbD assessment (Caldeira et al., 2022; Abbate et al., 2024; Garmendia Aguirre et al., 2025), methodologies encompassing all relevant processes and scales are not yet available (Caldeira et al., 2023; Abbate et al., 2024; Garmendia Aguirre et al., 2025).

To fully enable chemistry to become more sustainable it needs to be enlarged by starting with service and design, integrating systems thinking as well as alternative non-material-based business models.

3.2.2. Positioning SSbD among the current chemistry frameworks

The results from Chapter 3.1 show that the concepts of *Green Chemistry*, *Circular Chemistry*, *Chemistry within a Circular Economy*, and *Sustainable Chemistry* are all normative frameworks based on differing values (i.e. "greener is better", "circular is better", "more sustainable is better") whereas chemistry as a science is non-normative and independent of human value propositions. The industrial application of chemistry (the chemical sector with the chemical and pharmaceutical industries at its core) is based on the values of the current society, and thereby subject to change.

Sustainable Chemistry in its understanding and practice of chemistry is closest to sustainability and therefore, in the authors' opinion, is the ***framework giving guidance*** on how chemistry can comply with all sustainability dimensions (environmental, social, economic) for the preservation of our planet.

Green Chemistry provides a set of principles to contribute to greener synthesis, but its principles have severe limitations with respect to achieving sustainability in general. ***Circular Chemistry*** is a more holistic approach and adapted to the needs of a circular economy and therefore addresses the importance of considering end-of-life options (applying the ladder of circularity) already in the design. It addresses specific aspects of sustainability; however, it lacks a system thinking and the consideration of rebound effects, complexity of products and product flows, social aspects (see Chapter 3.1.2). While it is undoubtedly worth striving for a circular economy and a necessity to align chemical processes and products with its requirements, the limitations of a circular economy and of circularity itself from a thermodynamic point of view must also be acknowledged. The closely related concept ***Chemistry within a Circular Economy*** highlights the need to reduce complexity and toxicity of chemical products and designing for low entropy for products and products flows to contribute to sustainability. While all these concepts demonstrate how important design ('by-design') is as a preventive measure to target specific sustainability issues, none of these concepts address social or economic aspects in their principles (see Chapter 3.1.2 and Table 1) or take a holistic view on the backcloth of sustainability. Therefore, in the authors' opinion,

Key characteristics of Sustainable Chemistry	Sustainable Chemistry criteria categories	General Principles (GP) of Sustainable Chemistry	Golden Rules (GR) of Sustainable Chemistry	Revised SSbD Framework
1. Holistic	1. Climate and Ecosystem impacts	1. GP2: Quantitative development	1. ---	1. Safety and sustainability aspects are addressed with a holistic perspective throughout the innovation
2. Precautionary	2. Health and Safety Impacts	2. GP4: Action instead of reaction	2. GR1: only use substances which are not mentioned on lists of problematic substances	2. SSbD2 Minimise the use of hazardous chemicals/materials
3. System thinking	3. ----	3. ---	3. ---	3. The SSbD concept builds on multidisciplinary engagement of the life cycle actors and company experts
4. Ethical and social responsibility	4. Equity and Justice	4. ---	4. GR8 supply chain justice; GR9 societal and consumer benefit	4. The social-lifecycle assessment integrates ethical boundaries into the design process. SSbD9 Ensure responsible sourcing and minimise social risk
5. Collaboration & transparency	5. Transparency	5. ---	5. ---	5. The SSbD concept implies transparency of the assessment and traceability of the fulfilment of the principles throughout the entire innovation
6. Sustainable and responsible innovation	6. ----	6. GP5: Economic innovation	6. ---	6. Responsible innovation is embedded in the SSbD framework. Assessments consider the entire SSbD system including chemicals /materials, processes and products under study and their related life cycles.
7. Sound chemicals management	7. ----	7. ---	7. GR4: Avoid substances which require a high degree of risk management	7. SSbD5 Prevent and avoid hazardous emissions; SSbD6 Reduce exposure to hazardous substances
8. Circularity	8. Circularity	8. ---	8. GR5: Prefer substances from renewable resources;	8. SSbD7 Design for end-of- life; SSbD4 Use renewable sources
9. Green chemistry	9. ---	9. GP1: Qualitative development	9. GR3: avoid substances which are dangerous to human health and environment; GR7: Pay attention to a low energy, water consumption and waste	9. SSbD1 Material efficiency; SSbD3 Design for energy efficiency
10. Life cycle	10. ---	10. GP3: Comprehensive life cycle assessment	10. GR2: think of entire life cycle; GR6: Avoid long-distance transports	10. SSbD8 Consider the whole life cycle

Fig. 3. Graphical visualisation of Table 2 complemented by the revised SSbD framework (Garmendia Aguirre et al., 2025). Criteria, rules, and key characteristics of Sustainable Chemistry as defined by different organizations (ECOSChem 2023; UBA 2009, 2016; aligned to the Key Characteristics of Sustainable Chemistry (Kümmerer et al., 2021)).

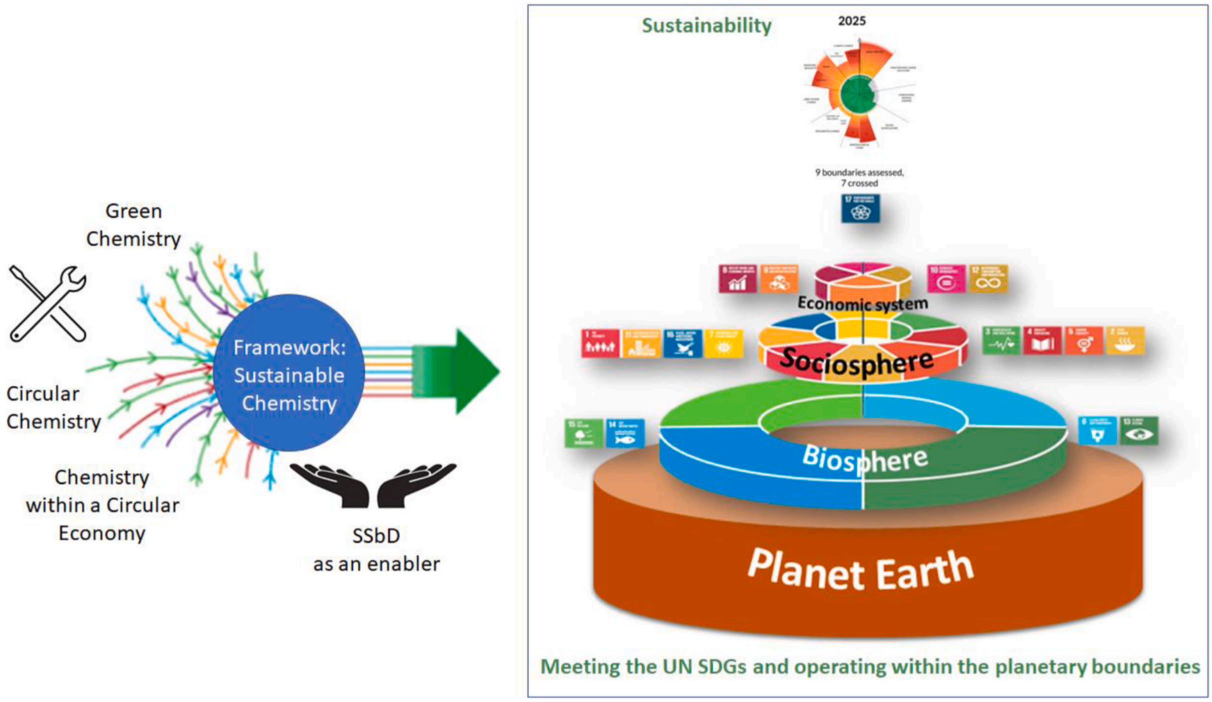

Fig. 4. Linking current chemistry frameworks with the United Nations (UN) Sustainable Development Goals (SDGs) and Planetary Boundaries. Green Chemistry, Circular Chemistry, and Chemistry within a Circular Economy are tools to move chemistry (as a sector) and its products towards more sustainability, while Sustainable Chemistry is the framework needed to achieve sustainability. SSbD is an enabler for Sustainable Chemistry to accelerate the transitions towards sustainability (right part was modified and adapted from Folke et al., 2016; Stockholm Resilience Centre, 2023).

Green Chemistry, Circular Chemistry, and *Chemistry within a Circular Economy* and their principles can be seen as ***tools for Sustainable Chemistry*** as they are suitable to target specific sustainability aspects (i.e. greener synthesis and circular value chains) but each of them has a too limited foci to achieve sustainability by its own (Fig. 2).

But how and where does SSbD fit into this picture? As shown in Chapter 3.2.1 SSbD is strongly interlinked with the discussed

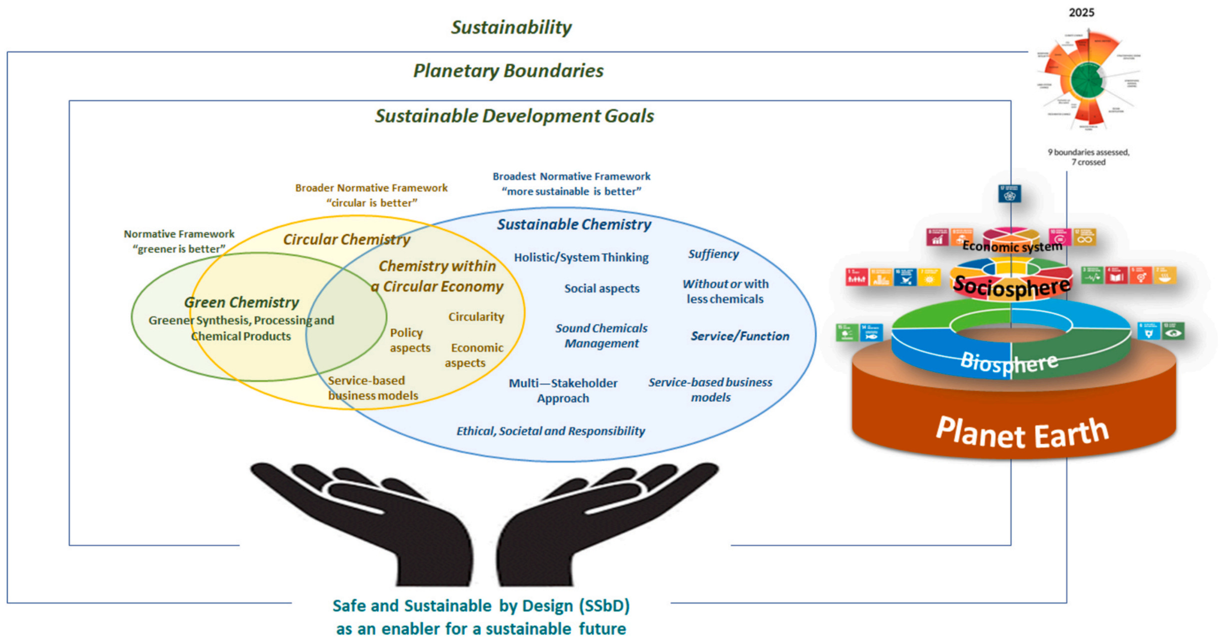

Fig. 5. Positioning SSbD among current chemistry and sustainability frameworks (right part was modified and adapted from Folke et al., 2016; Stockholm Resilience Centre, 2023).

chemistry concepts. For SSbD, greener synthesis (*Green Chemistry*), circular value chains (*Circular Chemistry and Chemistry within a Circular Economy*) are important objectives and tools (Fig. 2). The closest framework to SSbD is *Sustainable Chemistry* because of its systems thinking approach (Fig. 3). Nevertheless, it is important to point out that SSbD is an innovation approach, meaning all aspects of SSbD, i.e. covering the complete life cycle of a chemical, material, or product not just its value chain, need to be considered, implemented, and assessed already by the R&I team and downstream users when designing products (e.g., electronics, textiles, disinfectants, cosmetics or others). The recently published SSbD guidance by Cefic (2024) demonstrates how the SSbD design principles and assessment steps (Table 4) can be integrated into the stage-gate innovation process. This in mind, the authors consider ***SSbD as an enabler***[3] ***of Sustainable Chemistry*** to accelerate the transition towards sustainability from the design stage, thereby contributing to achieve the UN SDGs and ensuring humanity operates within the planetary boundaries (Figs. 4 and 5). SSbD is an important and, compared to *Green and Circular Chemistry,* a more comprehensive framework but cannot substitute *Sustainable Chemistry*.

3.2.3. Towards regenerative business and corporate strategies

Both *Sustainable Chemistry* and SSbD challenge chemists and designers to think of service and function first. Both concepts call not only for a change in i) how chemicals, materials, and products are produced (efficiency), but also for a change in ii) economic structures to reduce chemicals and materials flows (sufficiency), and iii) a balance between economic, social, and environmental factors over time (consistency) to transition towards more sustainability.

Operationalising these concepts therefore requires more than just the R&I teams to be supportive of this new way of thinking and working. There needs to be a drastic system change in business and corporate strategies towards a regenerative way of working that is planet-centred rather than economic-centred and that aims to do better with less rather than focusing on (economic) growth at all costs (Fig. 6). Only this transition enables an 'environment' with the broadest understanding of sustainability in which Sustainable Chemistry and SSbD can have their greatest impact.

4. Conclusions

In the mist of the triple crisis of climate change, biodiversity loss, and pollution, ensuring safety and sustainability is a necessity to operate within the planetary boundaries. The fields of sustainability-oriented innovation, safety, and sustainability itself (environmental, social and economic) need to come together in a holistic and lifecycle thinking approach as it is done through the application of SSbD throughout the lifecycle. This perspective explored where SSbD fits into the bigger picture of *Sustainable Chemistry*. This study shows that *Green Chemistry*, *Circular Chemistry* and *Chemistry within a Circular Economy* can be seen as tools to move chemistry (as a sector) and its products towards more sustainability, while *Sustainable Chemistry* is the framework defining their applicability domain to contribute sustainability in a sustainable manner. When positioning SSbD into this landscape, SSbD has the potential to act as an

[3] An enabler in this context can be described as a driver of radical change in the capabilities of a user or culture for accelerated impact.

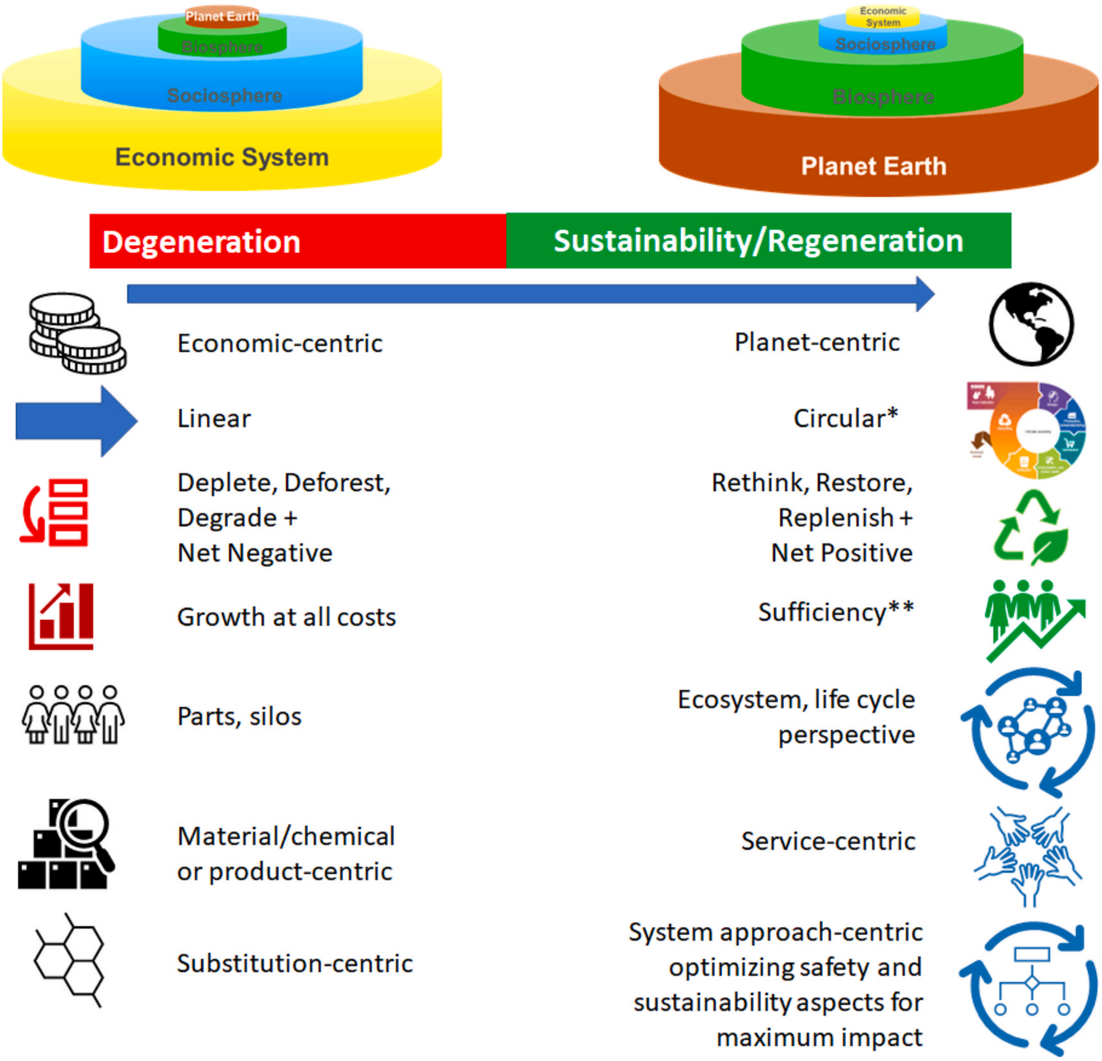

Fig. 6. Transition from an economic-centric system to a planet-centric system: Necessary characteristics of business and corporate strategies to move towards a sustainable future (* end-of-life consideration depending on the product's fate or sink: design for circularity if the product can be collected at the end of life or design for environmental degradation if the product is dispersed in the environment and cannot be collected; ** Sufficiency is not only "doing better with less", but producing more of those things that increase the social foundation and people's wellbeing, rather than producing marketable goods more efficiently. Sufficiency is a mindset that prioritises human and environmental well-being over material accumulation and includes practices such as minimalism, sharing economies, alternative non-material business models, and mindful consumption patterns that reduce overall resource use, energy needs, pollution, and waste generation.).

enabler of *Sustainable Chemistry* due to its integration within the companies' innovation process. Both *Sustainable Chemistry* and SSbD call not only for a change in how chemicals, materials, and products are produced (efficiency), but also for a change in economic structures (sufficiency), and a balance between economic, social, and environmental factors over time (consistency) to transition towards more sustainability. To fully enable chemistry to become fully embedded into sustainability it needs to be broadened by starting with service and design, integrating systems thinking as well as alternative non-material-based business models first. Operationalization of SSbD involves embedding SSbD into research and development (R&D) processes, regulatory frameworks, and industry practices. This will provide clear guidelines and incentives for sustainable innovation with a key focus on sustainable business models and on sustainable molecular, material, and product design. With this, SSbD acts as an enabler for *Sustainable Chemistry* and accelerates the transition towards more sustainable practices, achieving the SDGs and keeping inside the planetary boundaries and thus acts as an enabler for a sustainable future.

CRediT authorship contribution statement

Lya G. Soeteman-Hernández: Writing – review & editing, Writing – original draft, Validation, Methodology, Investigation, Funding acquisition, Conceptualization. **Christina Apel:** Writing – review & editing, Writing – original draft, Methodology, Investigation. **Emma Strömberg:** Writing – review & editing, Project administration, Funding acquisition. **Klaus Kümmerer:** Writing – review & editing, Writing – original draft, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scp.2026.102321.

Data availability

No data was used for the research described in the article.

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Further reading

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