

REPURPOSE

**Knowledge book on best
practices: SSbD polymer and
product development**



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Glossary of terms

Acronym	Definition
AI	Artificial Intelligence
BHET	Bis(2-hydroxyethyl) terephthalate
CEN	Comité Européen de Normalisation
CLP	Classification, Labelling and Packaging (Regulation)
CNCs	Cellulose Nanocrystals
CSS	Chemicals Strategy for Sustainability
DfD	Design for Disassembly / Design for Deconstruction
EC	European Commission
ECHA	European Chemicals Agency
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ED	Endocrine Disruptors
EMKG	Easy-to-use Workplace Control Scheme for Hazardous Substances
EUSES	European Union System for the Evaluation of Substances
FAIR	Findable, Accessible, Interoperable, Reusable
FDCA	2,5-Furandicarboxylic Acid
ILO	International Labour Organization
INRS	Institut National de Recherche et de Sécurité
IoT	Internet of Things
IP	Intellectual Property
JRC	Joint Research Centre
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MD	Molecular Dynamics (simulation)
ML	Machine Learning
MS	Member States

NAMs	New Approach Methodologies
NIR	Near-Infrared (reflectance spectroscopy)
PAT	Process Analytical Technology
PBT	Persistent, Bioaccumulative and Toxic
PEF	Polyethylene Furanoate
PET	Polyethylene Terephthalate
PFAS	Per- and Polyfluoroalkyl Substances
PHA	Polyhydroxyalkanoates
PLA	Polylactic Acid
PMT	Persistent, Mobile and Toxic
PPWR	Packaging and Packaging Waste Regulation
PVC	Polyvinyl Chloride
QSAR	Quantitative Structure–Activity Relationship
R&D / R&I	Research & Development / Research & Innovation
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RTOs	Research and Technology Organisations
SMEs	Small and Medium Enterprises
SoC	Substances of Concern
SSbD	Safe and Sustainable by Design
SVHC	Substances of Very High Concern
TEA	Techno-Economic Assessment
TRA	Targeted Risk Assessment
TRL	Technology Readiness Level
UV	Ultraviolet
VOCs	Volatile Organic Compounds
vPvB	Very Persistent Very Bioaccumulative
vPvM	Very Persistent Very Mobile

1 Introduction

This document originates from the Horizon Europe project **REPurpose** (G.A. n° 101057971; September 2022 – August 2026), which set out to upcycle local post-consumer plastic, paper and cardboard waste into new, functional REP polymers targeting high-value thermoplastics, with applications spanning the consumer goods, automotive, and building industries. The key point in developing these new polymers was doing so in line with the principles of the **Safe and Sustainable by Design (SSbD)** framework.

Building on this experience, the document is intended as a **knowledge book on SSbD** for polymer materials: it summarises what the project learned about applying the SSbD framework in practice, for a broad audience that includes: researchers and engineers, industry practitioners working on polymer innovation, who want to evaluate how to apply SSbD principles in their own material development processes, and policymakers interested in how the SSbD framework translates into practical guidance for the plastics and polymer sector.

The document has two complementary parts. The first part (**Chapters 2 to 13**) introduces the SSbD framework as defined by the European Commission and explains how its four principles - *functionality, safety, environmental sustainability, and circularity* - apply specifically to polymer design, synthesis, processing, product design, end-of-life management, and assessment tools.

The second part (**Chapters 14 to 16**) presents the challenges and solutions identified over the course of the REPurpose project: these were gathered from the project partners and reflect the practical, day-to-day obstacles encountered when trying to put SSbD principles into practice in polymer research and development, while the solutions capture the strategies the consortium found effective in addressing those obstacles. Detailed, partner-level accounts of these challenges are provided in the **Annex**, for readers who want to go beyond the summary presented in the main text.

1.1 Executive summary

Polymeric materials are essential to modern industry, but their production and use raise well-documented concerns around hazardous additives, climate impact, and end-of-life waste. The SSbD framework, introduced by the European Commission in 2022, offers a structured way to address these concerns by integrating safety, environmental sustainability, functionality, and circularity considerations from the earliest stages of material design, rather than retrofitting them after a product has been developed.

This knowledge book applies that framework specifically to polymer innovation. It first reviews how each SSbD principle plays out across the polymer value chain – from monomer selection and polymerization, through formulation, processing, product design, and end-of-life management, to the digital and assessment tools that support decision-making at each stage. It then incorporates the practical experience of the REPurpose project, to identify the main challenges encountered when applying SSbD to real polymer development work - *both general challenges common to the field and project-specific ones* - and the solutions the consortium developed in response.

The document closes with eight operational recommendations for practitioners: integrating sustainability from the earliest design stages; applying life cycle thinking throughout development; designing for circularity; minimizing hazardous additives; optimizing manufacturing for resource efficiency; using digital tools to accelerate innovation; fostering cross-sector collaboration; and investing in education and capacity building. These recommendations are intended as a practical starting point for any organization beginning its own SSbD journey in polymer materials.

2 Safe and Sustainable by Design (SSbD) framework for polymeric materials development

The development of polymeric materials has historically been driven by three principal objectives: **performance, cost efficiency, and scalability**.¹ Since the early expansion of the petrochemical industry in the mid-20th century, polymers have become indispensable^{2,3} materials across virtually all industrial sectors, including packaging, construction, automotive, electronics, healthcare, agriculture, and consumer goods. Their versatility arises from the ability to tailor polymer structures at the molecular level, enabling the design of materials with specific mechanical, thermal, chemical, and optical properties.

For decades, innovation in polymer science primarily focused on optimizing these performance attributes while ensuring that materials could be produced at a large scale and competitive cost. Advances in polymer chemistry, catalysis, and processing technologies allowed the rapid expansion of polymer production worldwide. Today, global plastic production exceeds **400 million tonnes annually**, and polymers represent one of the most widely used classes of materials in modern society.⁴

However, while polymers have provided significant technological and societal benefits, their widespread use has also generated important environmental and societal challenges.^{3,5} These challenges have become increasingly evident over the past two decades and have triggered growing concern among policymakers, scientists, industry stakeholders, and the general public.

¹¹ Callister, W. D., & Rethwisch, D. G. (2020). *Materials Science and Engineering: An Introduction* (10th ed.). John Wiley & Sons.

² Andrady, A. L., & Neal, M. A. (2009). Applications and societal benefits of plastics. *Philosophical Transactions of the Royal Society B: Biological Sciences*, 364(1526), 1977–1984. <https://doi.org/10.1098/rstb.2008.0304>

³ Geyer, R., Jambeck, J. R., & Law, K. L. (2017). Production, use, and fate of all plastics ever made. *Science Advances*, 3(7), e1700782. <https://doi.org/10.1126/sciadv.1700782>

⁴ Plastics Europe. (2024). *Plastics – the Fast Facts 2024: An analysis of European plastics production, demand and waste data*. <https://plasticseurope.org>

⁵ United Nations Environment Programme. (2023). *Turning off the Tap: How the world can end plastic pollution and create a circular economy*. Nairobi: UNEP.

In addition to environmental pollution, the **climate impact of polymer production** has become a major concern.⁶ The majority of conventional polymers are derived from fossil resources such as petroleum and natural gas.⁷ The extraction, refining, and conversion of these feedstocks into monomers and polymers require significant energy inputs and contribute to greenhouse gas emissions. As the global community works toward climate neutrality, reducing the carbon footprint of materials production has become a critical objective.

Another challenge relates to the **use of hazardous chemicals in polymer formulations**. Many polymer systems rely on additives⁸ such as plasticizers, stabilizers, flame retardants, pigments, and processing aids to achieve desired material properties. While these additives play important functional roles, some have raised concerns regarding toxicity, environmental persistence, and bioaccumulation. More information relative to these additives can be found in the public deliverable “D2.2. Additives inventory and roadmap II”. Substances such as certain phthalate plasticizers, brominated flame retardants, and heavy-metal stabilizers have been associated with adverse effects on human health and ecosystems. Consequently, regulatory agencies are increasingly restricting or phasing out substances identified as **substances of very high concern (SVHC)**⁹.

Furthermore, the **linear “take–make–dispose” model** historically associated with plastics has contributed to resource inefficiencies and waste generation.¹⁰ Many polymer products are designed without considering their end-of-life management, resulting in materials that are difficult to recycle or recover. Complex multi-layer structures, incompatible polymer blends, and additive-rich formulations can significantly hinder recycling processes. As a result, large quantities of plastic waste are currently landfilled or incinerated, representing a loss of valuable material resources.

These challenges have prompted governments and international organizations to develop new policy frameworks aimed at transforming the way materials are designed, produced, and managed throughout their life cycles. Within the European Union, one of the most important policy initiatives addressing these issues is the **European Green Deal**,¹¹ which aims to achieve climate neutrality and transition toward a sustainable and circular economy.

⁶ Zheng, J., & Suh, S. (2019). Strategies to reduce the global carbon footprint of plastics. *Nature Climate Change*, 9(5), 374–378. <https://doi.org/10.1038/s41558-019-0459-z>

⁷ International Energy Agency. (2018). *The Future of Petrochemicals: Towards More Sustainable Plastics and Fertilisers*. Paris: IEA.

⁸ Groh, K. J., Backhaus, T., Carney-Almroth, B., Geueke, B., Inostroza, P. A., Lennquist, A., Leslie, H. A., Maffini, M., Slunge, D., Trasande, L., Warhurst, A. M., & Muncke, J. (2019). Overview of known plastic packaging-associated chemicals and their hazards. *Science of the Total Environment*, 651, 3253–3268. <https://doi.org/10.1016/j.scitotenv.2018.10.015>

⁹ European Chemicals Agency. Candidate List of substances of very high concern for Authorisation. <https://echa.europa.eu/candidate-list-table>

¹⁰ Ellen MacArthur Foundation. (2016). *The New Plastics Economy: Rethinking the future of plastics*. <https://ellenmacarthurfoundation.org>

¹¹ European Commission. (2019). *The European Green Deal*. COM(2019) 640 final. Brussels: European Commission.

As part of this broader strategy, the European Commission introduced the **Chemicals Strategy for Sustainability (CSS)**,¹² which calls for the development of chemicals and materials that are inherently safe and sustainable throughout their life cycle. A central concept emerging from this strategy is **Safe and Sustainable by Design**.

The SSbD framework represents a paradigm shift¹³ in materials innovation. Rather than addressing environmental or safety concerns only after a product has been developed or commercialized, SSbD encourages researchers and developers to integrate these considerations **from the earliest stages of material design**. The objective is to prevent risks before they occur by designing materials that minimize hazards, reduce environmental impacts, and enable circularity.

In practical terms, SSbD seeks to guide the development of chemicals, materials, and products that simultaneously satisfy **four key dimensions**: functionality, safety, environmental sustainability, and circularity. This holistic perspective ensures that materials deliver the required performance while minimizing risks to human health and ecosystems and facilitating resource efficiency.

For polymer innovation, this approach requires a fundamental change in how research and development activities are conducted. Traditionally, polymer development follows a performance-driven pathway in which new materials are first optimized for functionality, and environmental or safety considerations are evaluated later in the development process. In contrast, SSbD promotes **integrated design**, where safety, sustainability, and circularity criteria are evaluated alongside performance from the very beginning of the innovation process.

This proactive design philosophy has several implications for polymer research and development. For example, the selection of monomers and building blocks should consider not only polymerization efficiency and final material properties but also toxicity, environmental persistence, and potential degradation pathways. Similarly, polymer synthesis routes should aim to minimize energy consumption, reduce the use of hazardous reagents, and improve resource efficiency.

Another key aspect of SSbD in polymer development involves designing materials that are compatible with **circular economy strategies**. This may include using waste streams as a resource for developing polymers that can then be efficiently recycled, designing materials with reversible or dynamic bonds that enable repair or chemical recycling, or selecting additives that do not interfere with recycling processes.

Importantly, SSbD also emphasizes the use of **life cycle thinking**. This means evaluating the environmental and health impacts of materials across all stages of their life cycle, including raw material extraction, polymer synthesis, processing, product use,

¹² European Commission. (2020). Chemicals Strategy for Sustainability: Towards a Toxic-Free Environment. COM(2020) 667 final. Brussels: European Commission.

¹³ Caldeira, C., Farcas, R., Moretti, C., Mancini, L., Rauscher, H., Rasmussen, K., Riego Sintes, J., Sala, S., & others. (2022). Safe and Sustainable by Design chemicals and materials: Framework for the definition of criteria and evaluation procedure for chemicals and materials (EUR 31100 EN). Publications Office of the European Union. <https://doi.org/10.2760/404543>

and end-of-life management. Tools such as **life cycle assessment (LCA)**, hazard assessment, and circularity indicators are commonly used to support this evaluation.

For technology centers, industrial R&D laboratories, and innovation ecosystems, implementing SSbD offers several strategic advantages. First, it supports **regulatory compliance** by anticipating future restrictions on hazardous substances and aligning material development with evolving regulatory frameworks. As regulations related to chemical safety and environmental performance continue to tighten, proactive adoption of SSbD principles can reduce the risk of costly product redesigns or market withdrawals.

Second, SSbD can contribute to **reducing environmental impacts** by lowering greenhouse gas emissions, minimizing resource consumption, and preventing pollution. By integrating sustainability considerations early in the design process, companies can identify opportunities for improving energy efficiency, reducing waste, and increasing material recyclability.

Third, adopting SSbD principles can enhance **product differentiation and market competitiveness**. Consumers, regulators, and investors are increasingly prioritizing sustainability, and companies that develop safer and more sustainable materials may gain competitive advantages in emerging markets. Sustainable materials are becoming particularly important in sectors such as packaging, electronics, automotive, and consumer products.

Finally, SSbD encourages **innovation and collaboration across value chains**. Implementing the SSbD framework often requires multidisciplinary expertise, including polymer chemistry, toxicology, environmental science, process engineering, and data analysis. Technology centers and research organizations can play a crucial role by facilitating collaboration among industry partners, developing standardized methodologies, and supporting the translation of scientific advances into practical industrial solutions.

In summary, the Safe and Sustainable by Design concept represents a transformative approach to polymer innovation. By integrating safety, sustainability, and circularity considerations from the earliest stages of research and development, SSbD provides a framework for developing polymer materials that support both technological progress and environmental stewardship. As regulatory pressures and societal expectations continue to evolve, the adoption of SSbD principles will likely become an essential component of responsible and competitive materials development.

3 Commission Recommendation of 8.12.2022

The Commission Recommendation of 8.12.2022¹⁴ established a European assessment framework for Safe and Sustainable by Design (SSbD) chemicals and materials. This recommendation was the main reference document applied within the REPurpose project

¹⁴ <https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32022H2510>

to define our strategy. The Recommendation has been generated taking into consideration the following aspects:

- The EU Green Deal sets out four interlinked policy goals for the transition to a sustainable economy and society: climate neutrality, biodiversity protection, circular economy and a zero-pollution ambition for a toxic-free environment.
- The EU sustainable finance strategy aims to support the financing of the transition to a sustainable economy.
- The Taxonomy Regulation sets out four conditions that an economic activity must fulfil to qualify as environmentally sustainable. It sets out six environmental objectives.
- In the Chemicals Strategy for Sustainability – Towards a Toxic-Free Environment (the 'Chemicals Strategy'), the EC announced that it would develop SSbD criteria for chemicals & materials.
- The EU Parliament adopted a resolution on the Chemicals Strategy, stressing the need to develop SSbD criteria to prevent and control pollution, improve the tracing of hazardous chemicals in products, and promote their substitution by safer and more sustainable alternatives.
- The Circular Economy Action Plan¹⁵ states that the EC will support the substitution and elimination of hazardous substances through R&I.
- The EU Action Plan Towards Zero Pollution for Air, Water and Soil and the Proposal emphasize the commitment to ensure that chemicals & materials are as safe and sustainable as possible by design and during their life cycle.
- A first sector-specific reference to SSbD can be found in the EU Strategy for Sustainable and Circular Textiles, to substitute or minimize SoC (substances of concern).
- A 2020 Eurobarometer survey shows that 84% of Europeans are worried about the impact on their health of chemicals present in everyday products, and 90% are worried about the impact of chemicals on the environment.
- Several hundred substances have already been identified as SVHC under REACH, and many more could fall under the definition of SoC in the Proposal for a Regulation for setting ecodesign requirements for sustainable products.
- Transition to chemicals & materials that are SSbD, requires a common understanding of safety and sustainability to be successful.
- The envisaged framework should make it possible to comprehensively assess the safety and sustainability of chemicals & materials throughout their life cycle and support the design, development, production, and use of chemicals & materials that provide a desirable function or service while being safe and sustainable.
- The review of safety and sustainability dimensions, aspects, methods, indicators, and tools focuses mainly on chemical safety and environmental sustainability. Assessments of socioeconomic aspects may be necessary for promoting substitution.
- The aim is to be at the forefront of research and innovation, and to promote the use of the latest scientific knowledge.
- The framework should aim to become a global reference for innovation in pursuit of the green industrial transition; for substituting the production and use of SoC; for promoting the use of sustainable resources and feedstock for the production of chemicals & materials; for minimizing the impact of the production and use of chemicals & materials, throughout their life cycle, on the climate, on the environment,

¹⁵ European Commission. (2020). A new Circular Economy Action Plan: For a cleaner and more competitive Europe. COM(2020) 98 final. Brussels: European Commission.

and on human health; and for driving industry's and public authorities' R&I investments in the right direction.

- It proposes a European SSbD framework as a point of reference for member states (MS), industry, academia, research and technology organisations (RTOs) and bodies providing benchmarks.
- It sets a testing period for the framework with a voluntary reporting mechanism for MS and stakeholders, which must be revised at the latest by the end of the testing period.
- Greater public and private investments in providing safe and sustainable chemicals, and a greater capacity to innovate on the part of the chemicals industry, will be vital for developing new solutions and supporting both the green and digital transitions. The vision for 2030 should therefore ensure that future EU, national and international initiatives are grounded.
- To provide incentives for testing the framework and addressing SoC, the EC will support the testing period through actions in the Horizon Europe framework programme.
- The EC has also developed a Strategic Research and Innovation Plan to facilitate and support.
- The EC will continue promoting findable, accessible, interoperable and reusable (FAIR) data. It is also developing an EU common data platform on chemicals, EUCHEM, to facilitate the sharing, access and re-use of existing data.

This Recommendation proposes that a European framework for SSbD chemicals & materials is to be established for R&I activities. The envisaged framework consists of methods for assessing these aspects with the aim that the results obtained will make it possible to define SSbD criteria, including scoring systems and thresholds. It is addressed to MS, industry, including SMEs, academia, and RTOs that work on the development of chemicals and materials, and encourages them to refer to the framework in relevant policy or strategy documents. It also encourages to report to the EC on the implementation of this Recommendation during the testing period and describes that the EC will make a reporting template available. The principles underpinning the SSbD framework are presented in **Figure 1**.

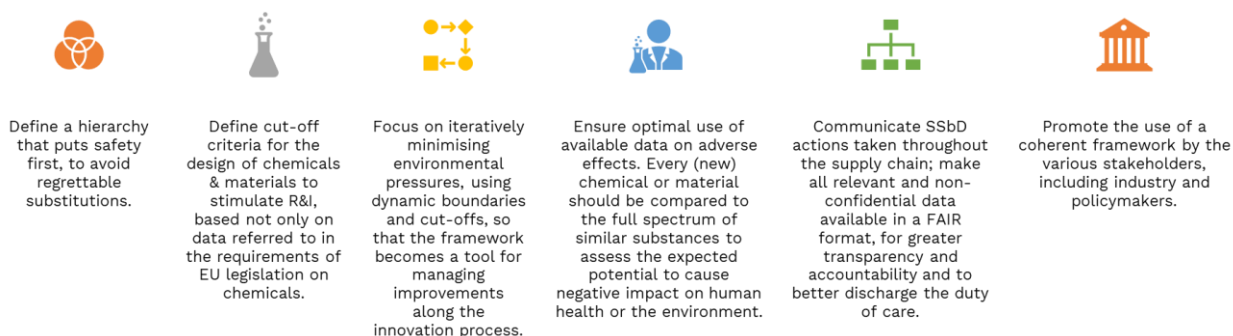


Figure 1. Principles underpinning the SSbD framework.

The SSbD framework can be applied to the development of new chemicals and materials, or to the reassessment of existing ones:

- i) to support the redesign of their production processes to make them safer and more sustainable by evaluating alternative processes, or
- ii) to compare them using the SSbD criteria (*e.g.*, for innovation by substitution with performing chemicals or materials or for selection in downstream applications).

It consists of 2 stages:

- i) Stage 1: (re)design stage, and
- ii) Stage 2: a safety and sustainability assessment across the different steps in the life cycle of a chemical or material, considering functionality and end-use(s).

It can help with the stages of the innovation process (design, planning, experimental testing and prototyping) where decisions are taken. It should start as early as possible to ensure that SSbD principles are being applied to a chemical or material's design. After that, the assessment should be done iteratively, at the subsequent stages of development, as more information gradually becomes available. The framework should allow for flexibility in its implementation, to ensure alignment with horizontal or product specific legislations or with regulatory exemptions.

a) Stage 1. The (re)design stage, at which guiding design principles are proposed to support the design

- (1) molecular design, to design new chemicals and materials based on their chemical structure;
- (2) process design, to make the production process safer and more sustainable, both for chemicals and materials being developed and for existing chemicals and materials;
- (3) product design, where the results of the SSbD assessment support the selection of the chemicals or materials to meet the functional demands of the final product in which they are used.

b) Stage 2: Safety and sustainability assessment (four steps) (Figure 2):

- ✓ Step 1 – Hazard assessment (intrinsic properties): to understand the hazard profile (human health, environment and physical hazards) of the materials. REACH and CLP are the most relevant regulations to be considered here. The three main hazard categories are:
 - 1. intrinsic hazardous properties relevant to human health (human health hazards);
 - 2. intrinsic hazardous properties relevant to the environment (environmental hazards);
 - 3. hazard physical properties (physical hazards).

Classification for SSbD assessment can already consider further hazard classes like: PBT (persistent, bioaccumulative and toxic), vPvB (very persistent very bioaccumulative), PMT (persistent, mobile and toxic), vPvM (very persistent very mobile) and ED (endocrine disruptors).

As the information available for new chemicals/materials could be limited at the beginning, a tiered approach is beneficial to be able to characterise hazards as early as possible by using new approach methodologies (NAMs).

- ✓ Step 2 – Human health and safety aspects of production and processing: assesses the human health and safety aspects of the production and processing of the chemical or material in question. Production means the production process from raw material extraction to the production of the chemical or material, including recycling or waste management. The goal is to assess whether the production and processing pose any risk to workers, in line with, or beyond, EU Occupational Health and Safety directives. A tiered approach can be applied to estimate the potential risk of exposure and the expected risk of exposure, for example: TRA tool developed by the European Centre for ECETOC, Chesar, ILO, German Hazardous Substances Column Model, supported by the “Easy-to-use Workplace Control Scheme for Hazardous Substances” (EMKG) tool, INRS model, Dutch Stoffenmanager model, Belgian REGETOX model.
- ✓ Step 3 – Human health and environmental aspects in the final application phase: assesses the hazards and risks of the final application to human health or the environment. To estimate exposure, it is important to identify/describe the application and define the use conditions (frequency and duration, amount, conditions and instructions for use). It is recommended to apply ECHA guidance (Chapter R12 Use description 21) as a starting point to define the use (categories of use). The chemical safety assessment and reporting tool (Chesar) is another tool recommended. For carrying out the exposure assessment, exposure estimation tools are included: ECETOC TRA tool for workers’ and for consumers’ exposure estimation, EUSES for environmental exposure estimation. Use maps, developed by industry sectors, collect information on the uses and the conditions of use of chemicals in their sector in a harmonised and structured way. Tools from higher tiers (ConsExpo) or sector specific tools developed by industry for assessing specific product types and articles can also be used.
- ✓ Step 4 – Environmental sustainability assessment: along the entire chemical/material life cycle by means of an LCA, assessing several impact categories such as climate change and resource use. Toxicity and ecotoxicity are also considered, referring to impacts due to life cycle emissions to humans and the environment via environmental compartments (e.g., soil, water, air), including mobility between compartments and not via direct exposure (covered in Step 3). The underlying models and characterisation factors¹⁶, should be applied.

¹⁶ <https://epplca.jrc.ec.europa.eu/LCDN/developerEF.xhtml>

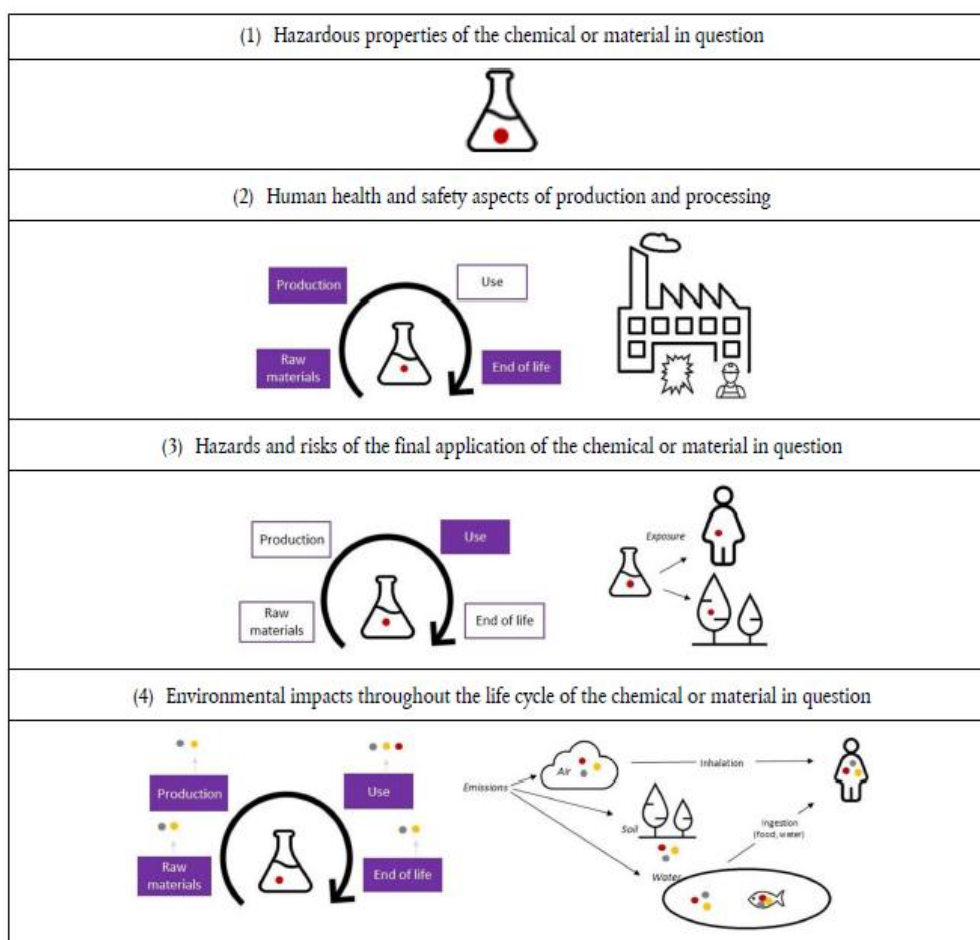


Figure 2. Illustration of the safety and sustainability aspects of the chemical or material covered by the safety and sustainability assessment. Coloured boxes indicate which life cycle stage is covered. The red dot refers to the chemical or material being assessed, while the yellow and grey dots refer to all the other substances emitted during its life cycle (e.g., other toxic chemicals emitted during the extraction of raw material or as a result of the energy used in the production process). Source: ¹⁴

The recommended data sources to support the safety and sustainability assessment suggested in this Recommendation are summarized in **Figure 3**.



Figure 3. Overview of data sources to support the safety and sustainability assessment.

4 SSbD principles applied to polymers

As introduced in Chapter 2, the **Safe and Sustainable by Design** framework provides a structured approach to guide the development of chemicals and materials that meet societal needs while minimizing risks to human health and the environment. Applied to polymer, this approach introduces a holistic design philosophy that integrates multiple dimensions of sustainability, from **functionality** to **safety, environmental sustainability, and circularity** throughout the entire life cycle of polymer materials and products.

These four principles are closely interconnected and should not be treated as independent criteria. A polymer material that performs well but poses health risks, generates significant environmental impacts, or cannot be recycled, cannot be considered fully sustainable. Consequently, SSbD requires that material developers evaluate trade-offs between these principles and adopt design strategies that balance performance with safety and sustainability goals.

4.1 Functionality

The first principle of SSbD is **functionality**, which ensures that materials fulfill their intended purpose and performance requirements. For polymer materials, functionality encompasses a wide range of properties that depend on the intended application. These properties may include mechanical strength, toughness, flexibility, thermal stability, chemical resistance, barrier performance, optical transparency, electrical conductivity, or biocompatibility.

For example, polymers used in packaging applications must often provide excellent barrier properties to protect food products from oxygen, moisture, and contaminants. In contrast, polymers used in automotive or construction applications must exhibit high mechanical strength and durability to withstand mechanical stress and environmental exposure. Medical polymers must meet stringent requirements related to sterility, biocompatibility, and chemical stability.

Ensuring functionality remains essential within the SSbD framework because materials that do not meet performance expectations may lead to premature failure, product replacement, or increased resource consumption. In other words, a material that is environmentally benign but fails to perform adequately could ultimately generate greater environmental impacts if products must be replaced more frequently.

In polymer design, functionality is largely determined by molecular structure and polymer architecture. Factors such as monomer composition, molecular weight, crystallinity, crosslinking density, and chain flexibility all influence the final properties of the material. Advances in polymer chemistry and materials engineering have enabled scientists to tailor these characteristics with high precision, allowing polymers to be optimized for specific applications.

Within the SSbD framework, functionality must therefore be considered alongside safety and sustainability considerations. The challenge lies in designing polymers that maintain high performance while minimizing environmental and health impacts.

4.2 Safety for Human Health and the Environment

The second core principle of SSbD is **safety**, which aims to minimize risks associated with chemical exposure and environmental contamination. In polymer systems, safety considerations extend beyond the polymer itself to include all substances involved in the material's life cycle. These include monomers, catalysts, solvents, additives, processing aids, degradation products, and potential impurities.

Historically, certain chemicals used in polymer production or formulation have raised concerns regarding toxicity and environmental persistence. Examples include certain phthalate plasticizers, brominated flame retardants, heavy metal stabilizers, and some residual monomers. Exposure to these substances may occur during manufacturing processes, product use, or waste management activities.

The SSbD framework encourages the early identification and elimination of **hazardous substances**, particularly those classified as substances of very high concern (SVHC) under European chemical regulations. Substituting hazardous chemicals with safer alternatives is a key strategy for reducing health and environmental risks.

In addition to intrinsic chemical hazards, safety considerations must also account for **exposure pathways**. For polymer-based products, exposure may occur through various mechanisms, including migration of additives from packaging materials, release of volatile substances, abrasion-generated microplastics, or degradation products formed during environmental weathering.

Assessing safety, therefore, requires a comprehensive evaluation of both hazard and exposure. Computational tools such as **quantitative structure–activity relationship (QSAR) models**, predictive toxicology platforms, and chemical databases can support early hazard screening during material design. Experimental testing methods, including in vitro toxicology and ecotoxicity studies, may also be required to evaluate potential risks.

By integrating safety assessments early in the innovation process, polymer developers can avoid the costly redesign of materials that may later be identified as hazardous or subject to regulatory restrictions.

4.3 Environmental Sustainability

The third principle of SSbD focuses on **environmental sustainability**, which involves minimizing environmental impacts associated with the production, use, and disposal of polymer materials. This principle encourages developers to consider the full life cycle of materials and to identify opportunities for reducing resource consumption, emissions, and waste generation.

One major aspect of environmental sustainability is the **carbon footprint** associated with polymer production. Conventional polymers are largely derived from fossil resources such as crude oil and natural gas, and their production can involve energy-intensive processes that generate significant greenhouse gas emissions. Transitioning to renewable feedstocks, improving energy efficiency, and adopting low-emission manufacturing technologies are important strategies for reducing climate impacts.

Resource efficiency is another important dimension of environmental sustainability. Polymer production requires not only fossil feedstocks but also water, energy, and various chemical reagents. Sustainable polymer design aims to reduce the consumption of these resources through improved process efficiency, the use of renewable raw materials, and the development of lightweight materials that require less material input for the same functionality.

Pollution prevention also plays a key role. Polymer production and processing can generate emissions into the air, water, and soil if not properly managed. Designing cleaner synthesis routes, reducing solvent use, and minimizing waste streams contribute to lowering environmental impacts.

Environmental sustainability assessments are commonly supported by **life cycle assessment (LCA)** methodologies, which quantify environmental impacts across different stages of a product's life cycle. LCA can evaluate indicators such as greenhouse gas emissions, energy demand, water consumption, acidification potential, and eutrophication potential. These assessments provide valuable insights that can guide material design decisions.

4.4 Circularity

The fourth principle of SSbD is **circularity**, which seeks to keep materials and resources in productive use for as long as possible. Traditional linear economic models follow a “take–make–dispose” pattern in which raw materials are extracted, converted into products, and eventually discarded as waste. Circular economy approaches aim to replace this model with systems that prioritize reuse, recycling, and resource recovery.

For polymer materials, achieving circularity requires careful consideration of material design and product architecture. Many conventional polymer products are difficult to recycle due to complex formulations, multilayer structures, or incompatible polymer blends.¹⁷ SSbD encourages developers to simplify material compositions and avoid design features that hinder recycling processes.

Design for recycling is one of the most important strategies for improving circularity. This may involve selecting widely recyclable polymer types, minimizing the number of additives, and avoiding substances that interfere with recycling technologies.

In addition to **mechanical recycling**, emerging technologies such as **chemical recycling and biological depolymerization** offer new opportunities for recovering polymer materials at the molecular level. Designing polymers with reversible bonds or depolymerizable structures can facilitate these recycling pathways.

Circularity also includes strategies such as **repairability, durability, and reuse**. Materials designed to last longer reduce the need for frequent replacement, thereby lowering resource consumption and waste generation.

¹⁷ Ragaert, K., Delva, L., & Van Geem, K. (2017). Mechanical and chemical recycling of solid plastic waste. Waste Management, 69, 24–58. <https://doi.org/10.1016/j.wasman.2017.07.044>

In some cases, biodegradable or compostable polymers may offer an alternative end-of-life pathway, particularly for applications where recycling is difficult. However, these materials must be carefully evaluated to ensure that they degrade safely under realistic environmental conditions.

4.5 Integrating the four principles

These four SSbD principles form a comprehensive framework for guiding polymer innovation. Achieving an optimal balance between these principles requires interdisciplinary collaboration among polymer chemists, materials engineers, toxicologists, environmental scientists, and product designers.

Their integration into the early stages of polymer development allows researchers to identify potential trade-offs and optimize materials accordingly. For instance, a polymer designed for high recyclability may require adjustments in additive selection to ensure safety and performance. Similarly, improving durability may reduce waste generation but could also influence degradation behavior at the end of life.

By adopting a holistic design approach that considers all four SSbD principles simultaneously, researchers and industry stakeholders can develop polymer materials that not only meet performance requirements but also contribute to a safer, more sustainable, and circular materials economy.

Putting these four principles into practice requires following the polymer value chain step by step. The chapters that follow examine each of these steps in turn: **polymer design** (Chapter 5); **synthesis** (Chapter 6); **formulation** (Chapter 7); **processing and manufacturing** (Chapter 8); **product design** (Chapter 9); and **circularity and end-of-life management** (Chapter 10). Chapters 11 to 13 then turn to the tools that support these decisions: environmental and safety assessment methods (Chapter 11), digital tools for polymer innovation (Chapter 12), and the overall SSbD innovation workflow that ties these stages together (Chapter 13).

5 Polymer design for safety and sustainability

The molecular design of polymers is a key determinant of their safety, environmental impact, and overall sustainability. Choices related to monomer selection, polymerization pathways, molecular architecture, and functional group incorporation affect material properties, toxicity, recyclability, degradation behavior, and compatibility with circular economy strategies. Increasing environmental awareness and regulatory pressures have therefore shifted polymer development toward materials that combine high performance with reduced hazards and environmental burdens, requiring a more comprehensive evaluation of both the chemical building blocks and the structural characteristics of the resulting polymers.

5.1 Selection of safer monomers

One of the most critical aspects of sustainable polymer design is the **selection of safer monomers and chemical building blocks**, compared to the substances of concern. Monomers form the fundamental units of polymer chains, and their chemical structure largely determines both the properties of the polymer and the potential risks associated with its production and degradation.

Within the SSbD framework, monomers should ideally meet several criteria related to safety and sustainability. First, they should exhibit **low intrinsic toxicity** to humans and ecosystems. This involves avoiding molecular structures associated with carcinogenicity, mutagenicity, reproductive toxicity, or endocrine disruption. Second, monomers should display **low environmental persistence** and minimal potential for bioaccumulation. Chemicals that remain in the environment for extended periods or accumulate in living organisms may pose long-term ecological risks.

Another important consideration is the **reactivity and conversion efficiency** of monomers during polymerization. High conversion rates minimize the presence of residual monomers in the final polymer product, thereby reducing the risk of exposure during product use. Residual monomers are a common concern in certain polymer systems, particularly when polymerization processes are not optimized or when monomers exhibit limited reactivity.

In addition to safety considerations, the SSbD approach also encourages the use of **renewable or bio-based feedstocks** when they can provide comparable performance and environmental benefits. Bio-based monomers derived from biomass, agricultural residues, or industrial by-products offer opportunities to reduce reliance on fossil resources and decrease greenhouse gas emissions associated with raw material extraction.

Several bio-based building blocks have gained significant attention in recent years as potential alternatives to conventional petrochemical monomers.¹⁸ One example is **2,5-furandicarboxylic acid (FDCA)**,¹⁹ which can be produced from carbohydrate-derived intermediates such as hydroxymethylfurfural. FDCA has been proposed as a replacement for terephthalic acid in polyester production and is used to synthesize polymers such as polyethylene furanoate (PEF),²⁰ which exhibit excellent barrier properties and improved thermal performance compared with traditional polyethylene terephthalate (PET).

¹⁸ Isikgor, F. H., & Becer, C. R. (2015). Lignocellulosic biomass: A sustainable platform for the production of bio-based chemicals and polymers. *Polymer Chemistry*, 6(25), 4497–4559. <https://doi.org/10.1039/C5PY00263J>

¹⁹ Sajid, M., Zhao, X., & Liu, D. (2018). Production of 2,5-furandicarboxylic acid from 5-hydroxymethylfurfural: A review. *Green Chemistry*, 20(24), 5427–5453. <https://doi.org/10.1039/C8GC02680G>

²⁰ de Jong, E., Dam, M. A., Sipos, L., & Gruter, G.-J. M. (2022). The road to bring FDCA and PEF to the market. *Polymers*, 14(5), 943. <https://doi.org/10.3390/polym14050943>

Another promising molecule is **levulinic acid**,^{21, 22} which can be derived from lignocellulosic biomass through acid-catalyzed conversion processes. Levulinic acid and its derivatives serve as versatile intermediates for producing polymer precursors, plasticizers, and solvents. Similarly, **itaconic acid**,²³ produced through microbial fermentation of sugars, offers a renewable alternative to acrylic acid and can be used to synthesize bio-based polyesters, polyamides, and specialty polymers.²⁴

Lactic acid, derived from the fermentation of carbohydrates, is perhaps one of the most well-known bio-based monomers.²⁵ It serves as the precursor for **polylactic acid (PLA)**,²⁶ a biodegradable polyester widely used in packaging, biomedical applications, and additive manufacturing. The development of PLA illustrates how bio-based monomers can support the transition toward more sustainable polymer systems when combined with efficient production technologies and appropriate end-of-life management strategies.

The adoption of bio-based monomers must nevertheless be evaluated carefully through life cycle assessments to ensure that their production does not introduce unintended environmental burdens such as excessive land use, water consumption, or agricultural emissions. Therefore, the sustainability of renewable feedstocks depends not only on their origin but also on the efficiency and environmental performance of their production processes.

5.2 Engineering polymer architecture

Beyond the selection of monomers, the **molecular architecture of polymer chains** plays a critical role in determining material behavior, safety, and environmental performance. Polymer architecture refers to the structural arrangement of monomer units and the overall topology of the polymer chain, including linear, branched, crosslinked, or network structures.

Polymer architecture can be deliberately engineered to enhance sustainability outcomes. One important strategy involves incorporating **degradable chemical linkages** into the polymer backbone. Functional groups such as esters, carbonates, anhydrides, or imines can introduce points of chemical vulnerability that allow controlled degradation under specific environmental conditions. These degradable linkages may facilitate

²¹ Kang, S., Fu, J., & Zhang, G. (2018). From lignocellulosic biomass to levulinic acid: A review on acid-catalyzed hydrolysis. *Renewable and Sustainable Energy Reviews*, 94, 340–362. <https://doi.org/10.1016/j.rser.2018.06.016>

²² Christensen, M. L., Warmuth, H., & Cumming, H. (2020). Levulinic acid: A sustainable platform chemical for novel polymer architectures. *Polymer Chemistry*, 11(25), 4068–4081. <https://doi.org/10.1039/D0PY00274A>

²³ Kuenz, A., Gallenmüller, Y., Willke, T., & Vorlop, K.-D. (2012). Microbial production of itaconic acid: Developing a stable platform for high product concentrations. *Applied Microbiology and Biotechnology*, 96, 1209–1216. <https://doi.org/10.1007/s00253-012-4221-y>

²⁴ Robert, T., & Friebe, S. (2016). Itaconic acid—A versatile building block for renewable polyesters with enhanced functionality. *Green Chemistry*, 18(10), 2922–2934. <https://doi.org/10.1039/C6GC00605A>

²⁵ Komesu, A., de Oliveira, J. A. R., Martins, L. H. S., Maciel, M. R. W., & Maciel Filho, R. (2017). Lactic acid production to purification: A review. *BioResources*, 12(2), 4364–4383. <https://doi.org/10.15376/biores.12.2.Komesu>

²⁶ Inkinen, S., Hakkarainen, M., Albertsson, A.-C., & Södergård, A. (2011). From lactic acid to poly(lactic acid): Characterization and analysis of PLA and its precursors. *Biomacromolecules*, 12(3), 523–532. <https://doi.org/10.1021/bm101302t>

biodegradation, hydrolysis, or enzymatic/chemical recycling processes that enable the recovery of valuable materials at the end of a product's life cycle.

For example, polyesters and polycarbonates contain hydrolysable bonds that can be broken down through chemical recycling processes or environmental degradation pathways. Designing polymers with such linkages can therefore contribute to improved end-of-life management and reduce long-term environmental persistence.

Another promising approach involves the use of **dynamic covalent chemistry**, which introduces reversible chemical bonds into polymer networks. Dynamic bonds can break and reform under specific stimuli such as heat, light, or changes in pH. This property enables materials to exhibit self-healing behavior, reshaping capabilities, or recyclability even when they possess crosslinked structures traditionally considered non-recyclable. Materials based on dynamic covalent chemistry, sometimes referred to as **vitrimer**s or adaptable polymer networks, represent an important innovation in sustainable polymer design. These materials combine the mechanical robustness of thermosets with the re-processability of thermoplastics, offering new opportunities for extending product lifetimes and improving material recovery.

5.3 Structural parameters influencing sustainability

In addition to chemical composition, several structural parameters of polymer chains influence both performance and sustainability. These include **molecular weight distribution, crystallinity, branching, and crosslink density**.

Molecular weight affects mechanical strength, processability, and degradation behavior. High molecular weight polymers typically exhibit superior mechanical performance but may be more difficult to recycle or degrade. Conversely, lower molecular weight materials may be easier to process or chemically recycle, but may not provide the required performance for certain applications.

Crystallinity is another important factor influencing material properties. Highly crystalline polymers often exhibit improved barrier properties, chemical resistance, and mechanical strength. However, increased crystallinity can also affect biodegradability and recycling behavior by limiting the accessibility of degradation agents or chemical reagents.

Branching and crosslink density determine the rigidity and dimensional stability of polymer materials. Highly crosslinked networks provide excellent mechanical and thermal resistance but are traditionally difficult to recycle due to their permanent network structure. The development of dynamic or reversible crosslinking systems offers promising solutions to address this challenge.

Optimizing these structural parameters requires balancing competing objectives related to performance, safety, and sustainability. Advanced characterization techniques and computational modeling tools can support this optimization process by providing insights into structure-property relationships and predicting material behavior.

5.4 Integrating molecular design with sustainability objectives

Ultimately, the design of polymers for safety and sustainability requires a **systems-level perspective** that integrates molecular design with broader environmental and societal considerations. Polymer scientists must evaluate not only the intrinsic properties of materials but also the processes used to produce them, the conditions under which they are used, and the pathways available for their recovery or disposal.

By incorporating safer monomers, renewable feedstocks, degradable linkages, and adaptable polymer architectures, researchers can develop materials that align with SSbD principles while maintaining the functionality required for modern applications. Advances in green chemistry, biotechnology, and materials science continue to expand the range of sustainable polymer building blocks and design strategies available to researchers.

As polymer science evolves, the integration of safety and sustainability considerations into molecular design will become increasingly important. Through careful selection of monomers and thoughtful engineering of polymer architectures, it is possible to create materials that meet performance demands while contributing to a more sustainable and circular materials economy.

6 Sustainable polymer synthesis

The sustainability of polymer materials is determined not only by their chemical composition but also by the **processes used to synthesize them**. Polymer production is traditionally associated with significant energy consumption, the use of organic solvents, hazardous catalysts, and the generation of by-products or waste streams. Within the SSbD framework, polymer synthesis must therefore be re-evaluated to reduce environmental impacts while maintaining high productivity and material quality.

Sustainable polymer synthesis focuses on **minimizing resource consumption, reducing emissions, and improving process efficiency**. This objective can be achieved through several complementary strategies, including the adoption of green polymerization techniques, the reduction or elimination of solvents, the use of safer catalysts, and the implementation of process intensification technologies. By integrating these approaches, polymer manufacturers can significantly reduce the environmental footprint associated with polymer production.

6.1 Green polymerization techniques

Green polymerization methods represent a key strategy for improving the sustainability of polymer synthesis. These approaches aim to operate under milder reaction conditions, reduce the use of hazardous chemicals, and improve reaction efficiency. One particularly promising area is **enzymatic polymerization**, which utilizes biological catalysts such as lipases or other enzymes to facilitate polymer formation.

Enzymatic polymerization offers several environmental advantages compared with conventional catalytic systems. Enzymes typically operate under relatively mild temperatures and pressures, reducing the energy requirements of the polymerization process. In addition, enzymatic catalysts often exhibit high selectivity, which minimizes the formation of unwanted by-products and improves overall reaction efficiency. These processes are particularly attractive for the synthesis of polyesters and polyamides derived from bio-based monomers.

Another important advantage of enzymatic systems is their compatibility with **renewable feedstocks**. Enzymatic reactions can often be performed in aqueous or environmentally benign media, reducing the need for toxic solvents. Furthermore, enzymes are biodegradable and can sometimes be recovered or reused, further improving the sustainability profile of the process.

Despite these advantages, enzymatic polymerization still faces challenges related to catalyst stability, reaction rates, and scalability. Continued advances in enzyme engineering and biotechnology are expected to improve the industrial feasibility of these processes.

6.2 Solvent-free polymerization

One of the most effective strategies for reducing environmental impacts in polymer synthesis is the **elimination or reduction of the use of organic solvents**. Many traditional polymerization processes rely on organic solvents to dissolve monomers, control reaction temperatures, or facilitate heat transfer. However, solvents can contribute significantly to environmental emissions, particularly in the form of volatile organic compounds (VOCs).

Solvent-free polymerization techniques provide an attractive alternative. In these processes, monomers are polymerized in the **melt phase** or through solid-state reactions without the use of additional solvents. Eliminating solvents offers several advantages, including reduced emissions, simplified purification steps, and improved process safety.

One widely used solvent-free method is **melt polymerization**, in which monomers are heated above their melting points and polymerized directly in the molten state. Melt polymerization is commonly used for the production of polyesters, polyamides, and polycarbonates. Because no solvent removal is required, the process is generally more energy-efficient and generates fewer waste streams.

Another solvent-free approach involves **reactive extrusion**, where polymerization or polymer modification reactions occur within an extrusion process. Reactive extrusion integrates chemical reactions with polymer processing operations, enabling continuous production and improved process efficiency. This method is particularly useful for polymer functionalization, chain extension, grafting reactions, and the synthesis of certain types of copolymers. Additionally, this technology **reduces energy consumption** because it involves processes of only a few minutes reaction time.

By combining polymerization and processing into a single step, reactive extrusion can significantly reduce energy consumption, processing time, and equipment requirements.

6.3 Photopolymerization

Photopolymerization represents another promising route for sustainable polymer synthesis, particularly in applications such as coatings, adhesives, inks, and advanced functional materials. In photopolymerization processes, polymerization is initiated by light - *typically ultraviolet (UV) or visible radiation* - rather than by thermal activation.

One of the key advantages of photopolymerization is its **high energy efficiency**. Because the reaction is initiated by light rather than heat, the process can often be conducted at ambient temperatures, reducing energy consumption. In addition, photopolymerization reactions can occur extremely rapidly, allowing high production rates.

Photopolymerization also offers excellent **spatial and temporal control** over the polymerization process. The reaction can be initiated precisely where and when light is applied, making it particularly useful for additive manufacturing technologies such as stereolithography and other forms of 3D printing.

Another sustainability advantage is the potential for **solvent-free formulations**, which are common in UV-curable coatings. These systems often consist of reactive oligomers and monomers that polymerize directly upon irradiation, eliminating the need for solvent evaporation.

Nevertheless, the environmental performance of photopolymerization systems also depends on the selection of photoinitiators and reactive monomers. Some photoinitiators may pose toxicity concerns, and therefore, their selection should be carefully evaluated.

6.4 Catalyst selection and green catalysis

Catalysts play a central role in polymer synthesis, influencing reaction rates, product selectivity, and energy efficiency. However, some conventional catalytic systems rely on heavy metals or toxic reagents that may pose environmental or health risks. The selection of catalysts should prioritize **high activity, selectivity, low toxicity, and recyclability**.

Recent advances in **organocatalysis** offer promising alternatives to traditional metal-based catalysts. Organocatalysts are small organic molecules capable of promoting polymerization reactions without the need for metal species. These catalysts are often less toxic and may reduce the risk of metal contamination in polymer products.

Another important development involves the use of **biocatalysts**, such as enzymes, which can catalyze polymerization reactions under environmentally benign conditions. Enzyme-based catalysts are typically biodegradable and may provide excellent selectivity for specific reactions.

Heterogeneous catalytic systems also contribute to sustainable polymer synthesis because they can often be **recovered and reused**, reducing catalyst consumption and waste generation. Advances in catalyst immobilization techniques allow catalysts to be anchored onto solid supports, facilitating their separation from reaction mixtures.

6.5 Process intensification

In addition to improvements in polymerization chemistry, **process intensification** technologies offer significant opportunities to enhance the sustainability of polymer synthesis. Process intensification involves redesigning chemical processes to improve efficiency, reduce energy consumption, and minimize waste.

One important strategy is the use of **continuous processing** instead of traditional batch reactions. Continuous reactors often provide improved heat and mass transfer, more precise reaction control, and higher productivity. Continuous polymerization processes are increasingly used in industrial polymer production because they allow more efficient use of resources and energy.

Reactive extrusion, as previously mentioned, is a key example of process intensification in polymer manufacturing. By combining chemical reactions with polymer processing, reactive extrusion reduces the need for multiple processing steps and improves overall efficiency.

Other emerging technologies include **microwave-assisted polymerization**, which uses microwave energy to heat reaction mixtures rapidly and uniformly. Microwave heating can accelerate reaction kinetics, reduce reaction times, and improve product yields.

Similarly, **flow chemistry and microreactor technologies** offer promising opportunities for improving polymer synthesis processes. These systems allow precise control of reaction conditions, enabling more efficient use of reagents and improved product consistency.

6.6 Toward more sustainable polymer manufacturing

The transition toward sustainable polymer synthesis requires the integration of multiple strategies that address both chemical and process-related aspects of polymer production. Green polymerization methods, solvent-free processes, safer catalysts, and advanced manufacturing technologies collectively contribute to reducing the environmental footprint of polymer production.

Implementing these approaches not only supports environmental objectives but can also improve process economics by reducing energy consumption, simplifying purification steps, and increasing production efficiency. As sustainability considerations become increasingly important in the chemical and materials industries, the adoption of sustainable polymer synthesis strategies will play a crucial role in the development of next-generation polymer materials aligned with SSbD principles.

7 Sustainable polymer formulation

Polymer materials used in real-world applications are rarely composed solely of a polymer matrix. Instead, they are typically formulated with a wide variety of **additives and fillers** that are incorporated to tailor the physical, chemical, and functional properties of the final material. These additives play essential roles in improving processability, durability, mechanical performance, thermal stability, optical characteristics, flame resistance, and resistance to environmental degradation. As a result, polymer formulations can be complex systems in which the polymer backbone interacts with numerous additional components designed to optimize material performance for specific applications.

Despite their importance in achieving the desired functionality of polymer products, additives also represent one of the most significant sources of **safety and environmental concerns** in polymer systems. Many additives are small molecules that are not chemically bound to the polymer matrix, meaning they may migrate from the material during its service life or during disposal. This migration can lead to exposure of humans and ecosystems to potentially hazardous chemicals. Therefore, within the SSbD framework, careful consideration must be given to the selection, compatibility, and long-term behavior of additives used in polymer formulations (more information can be found in the public deliverable “D2.2. Additives inventory and roadmap II”).

Among the most common additive classes used in polymer materials are **plasticizers, stabilizers, flame retardants, pigments, antioxidants, lubricants, and fillers**. Plasticizers are widely used to increase flexibility and processability in polymers such as polyvinyl chloride (PVC), while stabilizers protect polymers from thermal or ultraviolet degradation. Flame retardants are incorporated to improve fire resistance, pigments provide color and aesthetic properties, antioxidants prevent oxidative degradation during processing and service life, and lubricants reduce friction between polymer chains and processing equipment, improving melt flow and preventing surface defects during extrusion or injection molding, and fillers are used to reinforce mechanical strength or reduce material costs.

Historically, several widely used additives have been associated with **toxicological or environmental concerns**. For example, certain **phthalate plasticizers** have been shown to exhibit endocrine-disrupting properties, leading to restrictions on their use in many consumer products such as toys, food packaging, and medical devices. Similarly, **brominated flame retardants**, which have been extensively used to improve fire resistance in plastics used in electronics and construction, have raised concerns due to their persistence in the environment and potential bioaccumulation in living organisms.

In response to these concerns, regulatory frameworks such as the European Union’s **REACH regulation** have identified numerous chemicals as **Substances of Very High Concern (SVHC)**. These substances may be subject to restrictions, authorization requirements, or phase-out initiatives. Consequently, sustainable polymer formulation increasingly focuses on identifying **safer alternatives** that maintain material performance while minimizing health and environmental risks.

Within the SSbD framework, additive selection should therefore prioritize substances with **favorable hazard profiles**, low persistence, and minimal bioaccumulation potential. This approach requires a combination of chemical hazard assessment, exposure evaluation, and life-cycle analysis. Computational tools and toxicological databases can assist researchers in screening potential additives and identifying safer substitutes during the early stages of material design.

Another critical aspect of sustainable polymer formulation is ensuring **compatibility between additives and the polymer matrix**. Additives that are poorly compatible with the polymer may segregate, volatilize, or migrate to the surface of the material over time. Migration is particularly problematic in applications involving direct contact with food, medical devices, or products used by children, where chemical exposure may occur through ingestion, inhalation, or dermal contact.

Additive migration can also occur during product aging, mechanical stress, or exposure to environmental conditions such as heat, light, or humidity. Therefore, improving additive compatibility with polymer matrices is essential for both safety and material durability.

One promising strategy for reducing additive migration involves the use of **reactive additives**. Unlike conventional additives that remain physically dispersed within the polymer matrix, reactive additives contain functional groups capable of chemically bonding to the polymer backbone during processing or polymerization. This chemical attachment significantly reduces the likelihood of additive leaching or volatilization.

Reactive additives have been developed for a variety of applications, including reactive plasticizers, stabilizers, and flame retardants. By becoming part of the polymer network, these additives can provide long-term stability while reducing potential exposure risks. In addition, reactive additives may improve the overall durability of polymer materials by preventing additive loss during product use or recycling.

In addition to improving the safety of additives, sustainable polymer formulation can also benefit from the incorporation of **bio-based fillers and reinforcement materials**. Natural materials derived from renewable biomass resources offer an attractive alternative to conventional mineral fillers such as talc, calcium carbonate, or glass fibers. Bio-based fillers often exhibit lower density and may provide environmental advantages by reducing dependence on non-renewable resources.

Examples of bio-based reinforcement materials include **natural fibers** such as flax, hemp, jute, and sisal. These fibers can be incorporated into polymer matrices to create lightweight composite materials with good mechanical strength. Such materials are increasingly used in sectors such as automotive manufacturing, where lightweight structures contribute to improved fuel efficiency and reduced greenhouse gas emissions.

Other promising bio-based fillers include **lignin, cellulose nanocrystals (CNCs), and nanofibrillated cellulose**. Lignin, a major component of plant biomass, can be used as a filler or antioxidant additive in polymer formulations. Cellulose-based nanomaterials exhibit high mechanical strength and large surface area, enabling them to reinforce polymers while improving barrier properties and thermal stability.

Another emerging bio-derived filler is **biochar**, which is produced through the pyrolysis of biomass. Biochar particles can improve mechanical performance, electrical conductivity, and thermal stability in certain polymer composites while also contributing to carbon sequestration.

In recent years, **nanomaterials** have also gained increasing attention as advanced additives capable of significantly enhancing polymer performance. Because of their extremely high surface area and unique physicochemical properties, nanomaterials can dramatically influence polymer behavior even when used in small amounts. However, the use of nanomaterials introduces new challenges related to **nanotoxicology and environmental safety**.

Ultimately, sustainable polymer formulation requires a **holistic approach** that integrates material performance with safety, environmental compatibility, and circularity considerations. By selecting safer additives, improving additive compatibility, incorporating renewable fillers, and carefully evaluating advanced materials such as nanomaterials, polymer scientists can develop formulations that support both functional performance and sustainability objectives.

As regulatory requirements and societal expectations continue to evolve, the development of safer and more sustainable polymer formulations will play a crucial role in the transition toward **responsible materials innovation and circular polymer systems**.

8 Processing and manufacturing

Polymer processing and manufacturing represent critical stages in the life cycle of polymer materials and significantly influence their overall environmental footprint. After polymer synthesis, raw polymer resins must be transformed into usable products through various **processing operations**, including extrusion, injection molding, blow molding, thermoforming, rotational molding, and compounding. These operations involve the application of heat, pressure, and mechanical forces to shape polymer materials into final products such as films, packaging, automotive components, consumer goods, and construction materials.

Although polymer processing technologies are highly optimized for industrial productivity, they can also be **energy-intensive** and generate environmental impacts associated with electricity consumption, material losses, and emissions. As global polymer production continues to increase, improving the sustainability of processing and manufacturing operations has become an important priority within the **SSbD** framework.

Sustainable polymer processing strategies focus on reducing **energy consumption, minimizing waste generation, improving resource efficiency, and optimizing process performance**. Advances in material science, equipment design, and digital technologies are enabling manufacturers to implement more environmentally responsible processing practices without compromising productivity or product quality.

8.1 Energy consumption in polymer processing

Polymer processing operations typically require the heating of polymer materials to temperatures ranging from 150°C to over 300°C, depending on the polymer type. Energy is consumed both for heating polymer melts and for driving mechanical equipment such as extruder screws, injection molding machines, and auxiliary systems. Consequently, polymer processing facilities can represent significant sources of industrial energy demand.

One effective strategy for improving sustainability in polymer manufacturing is the adoption of **low-temperature processing technologies**. Lower processing temperatures reduce the amount of thermal energy required to melt and shape polymers, thereby lowering energy consumption and greenhouse gas emissions associated with electricity generation. A similar approach that can achieve a reduction in energy consumption was previously mentioned with the technology of **reactive extrusion**, which involves a few minutes of processing.

Lower temperatures also offer additional advantages related to material stability. Many polymers and additives are susceptible to **thermal degradation** when exposed to high temperatures for extended periods. Degradation can lead to discoloration, loss of mechanical properties, formation of volatile compounds, and the generation of unwanted by-products. By processing materials at lower temperatures, manufacturers can preserve polymer integrity and improve product quality.

Advances in polymer chemistry have enabled the development of materials with improved **processability at lower temperatures**. For example, plasticizers, processing aids, and copolymer modifications can reduce melt viscosity, allowing polymers to flow more easily during processing. Similarly, improved screw designs in extrusion equipment allow better mixing and heat transfer, enabling efficient processing under milder thermal conditions.

8.2 Solvent-free compounding and processing

Another important strategy for sustainable polymer manufacturing involves the adoption of **solvent-free processing methods**. In many chemical processes, solvents are used to dissolve or disperse materials and facilitate mixing or chemical reactions. However, solvent use can introduce environmental and safety challenges, including emissions of volatile organic compounds (VOCs), solvent recovery requirements, and potential occupational exposure.

Polymer processing technologies such as **melt compounding and reactive extrusion** operate without the need for solvents. In melt compounding, polymers and additives are mixed in the molten state using mechanical shear forces within an extruder or internal mixer. This approach allows additives to be uniformly dispersed throughout the polymer matrix while eliminating solvent handling and evaporation steps.

Reactive extrusion extends this concept by allowing chemical reactions to occur directly within the extrusion process. Polymer modification, chain extension, grafting reactions, and compatibilization of polymer blends can be performed in a continuous process

without the need for solvents or additional reactors. By integrating chemical reactions with polymer processing, reactive extrusion reduces the number of processing steps, improves efficiency, and minimizes waste generation.

The elimination of solvents provides several environmental benefits. It reduces atmospheric emissions, lowers the need for solvent recovery systems, and simplifies purification processes. As a result, solvent-free processing is widely recognized as an important element of **green manufacturing in the polymer industry**.

8.3 Process integration and optimization

In addition to improvements in material formulation and equipment design, significant sustainability gains can be achieved through **integration and optimization**. Polymer processing systems consist of multiple interconnected components, including heating elements, motors, cooling systems, conveyors, and material handling equipment. Optimizing the interaction between these components can significantly reduce energy losses and improve overall process efficiency.

One common strategy involves the implementation of **heat recovery systems**. During polymer processing operations, large amounts of heat are generated and often dissipated as waste heat. Heat exchangers can capture this excess thermal energy and reuse it within the process, for example, by preheating incoming materials or supplying heat to other manufacturing operations. By recovering and reusing heat, manufacturers can significantly reduce their overall energy consumption.

Advanced **process control systems** also play an important role in improving sustainability. Modern polymer processing equipment is increasingly equipped with sensors that monitor key process variables such as temperature, pressure, screw torque, and material flow rates. These sensors provide real-time data that can be used to optimize processing conditions and minimize energy consumption.

Digital monitoring technologies, including **industrial Internet of Things (IoT) platforms**, allow manufacturers to analyze process data continuously and identify inefficiencies or deviations from optimal operating conditions. Predictive maintenance systems can detect early signs of equipment wear or malfunction, preventing unplanned downtime and reducing energy waste.

The integration of **data analytics and machine learning** into polymer processing operations is further enhancing the ability of manufacturers to optimize production processes. Machine learning algorithms can analyze large datasets to identify patterns that improve processing stability, reduce scrap rates, and enhance energy efficiency.

8.4 Water use and cooling systems

Water consumption represents another important environmental consideration in polymer manufacturing. Water is widely used in processing facilities for cooling equipment, controlling process temperatures, and cleaning machinery. For example, extrusion lines often rely on water baths to cool extruded products such as pipes, films, or profiles.

Traditional cooling systems may involve continuous water flows that discharge heated water after use, leading to high water consumption and potential thermal pollution. Sustainable manufacturing practices, therefore, emphasize the adoption of **closed-loop water systems**, in which water is continuously recycled within the facility.

In closed-loop systems, water is circulated through cooling towers or heat exchangers that dissipate heat before the water is reused in the process. This approach significantly reduces water consumption and minimizes wastewater discharge. Additionally, improved cooling technologies such as **air-cooled heat exchangers** or hybrid cooling systems can further reduce reliance on water resources.

Water management strategies may also include filtration systems that remove contaminants from processed water, allowing them to be reused multiple times without compromising equipment performance or product quality.

8.5 Toward sustainable polymer manufacturing

Improving the sustainability of polymer processing and manufacturing requires a combination of **technological innovation, process optimization, and resource management strategies**. Low-temperature processing technologies, solvent-free compounding methods, heat recovery systems, and digital monitoring tools all contribute to reducing the environmental footprint of polymer production.

In addition, the adoption of efficient water management systems and advanced manufacturing technologies supports the transition toward more sustainable and resource-efficient production processes.

As sustainability becomes an increasingly important consideration for industry and policymakers, polymer manufacturers are expected to adopt more energy-efficient and environmentally responsible production practices. Integrating these practices within the broader SSbD framework ensures that polymer materials are not only designed for safety and sustainability at the molecular level but also produced through manufacturing processes that minimize environmental impacts.

Through continued innovation in processing technologies and manufacturing strategies, the polymer industry can play a key role in advancing sustainable materials production while maintaining the high levels of performance and scalability required for modern applications.

9 Product design and performance

The design of polymer-based products plays a fundamental role in determining their environmental, economic, and social impacts throughout their life cycle. While material selection and manufacturing processes are critical components of sustainability, the **product design phase** ultimately determines how materials are used, how long products last, and how they are managed at the end of their life. Within the SSbD

framework, product design integrates material functionality with environmental responsibility, ensuring that polymer products deliver the required performance while minimizing negative environmental impacts.

Product designers must therefore balance **technical performance requirements with sustainability considerations**, including durability, resource efficiency, reparability, and recyclability. The design phase represents a critical opportunity to influence the entire life cycle of a product because many sustainability-related decisions—such as material choice, structural design, and component integration—are determined early in the development process. Decisions made during design can significantly affect manufacturing energy use, product longevity, maintenance requirements, and end-of-life management.

9.1 Design for durability

One of the most important principles of sustainable product design is **design for durability**. Products that maintain their functionality and structural integrity over extended periods reduce the need for frequent replacement, thereby lowering material consumption and waste generation. This approach directly contributes to resource efficiency by maximizing the useful life of materials and reducing the demand for new raw materials.

Durability in polymer products depends on several factors, including resistance to mechanical stress, thermal stability, resistance to ultraviolet (UV) radiation, and protection against environmental degradation. Many polymer products are exposed to harsh conditions during use, such as fluctuating temperatures, humidity, sunlight, chemical exposure, and mechanical wear. These factors can cause polymer degradation, leading to loss of mechanical strength, discoloration, embrittlement, or surface cracking.

To improve durability, designers often incorporate **stabilizing additives** such as UV stabilizers, antioxidants, and heat stabilizers that protect polymers from environmental degradation. In addition, selecting polymer materials with inherently high resistance to environmental stress - *such as high-performance engineering polymers* - can significantly extend product lifetimes.

Structural design also plays a key role in improving durability. Optimizing component geometry, reducing stress concentrations, and incorporating reinforcement materials can enhance mechanical performance and resistance to fatigue. In sectors such as automotive engineering, consumer electronics, and infrastructure, durable polymer components contribute to improved product reliability and reduced maintenance requirements.

However, durability must be balanced with considerations related to sustainability and end-of-life management. Extremely durable materials may persist in the environment if they are not properly recycled or recovered. Therefore, sustainable design aims to combine long product lifetimes with strategies that enable material recovery once the product reaches the end of its service life.

9.2 Design for deconstruction/disassembly

These approaches are closely linked to circular economy strategies because they facilitate the separation, repair, replacement, reuse, and recycling of materials at the end of a product's useful life. Design for Disassembly refers to the development of products in such a way that their components can be easily separated using non-destructive methods. This is especially relevant for polymer-based products used in sectors such as automotive, electronics, construction, and packaging, where complex assemblies often combine different materials, adhesives, coatings, or reinforcements that hinder recycling processes. In the context of polymer systems, **Design for Disassembly** (DfD) may involve reducing the number of polymer types within a product, avoiding permanent adhesives or inseparable multilayer structures, using reversible joining systems, designing modular components that can be independently replaced or repaired, facilitating material identification and separation during waste treatment. Similarly, **Design for Deconstruction** (DfD) expands this concept to larger systems and infrastructures, particularly in sectors such as construction and industrial equipment. The objective is to ensure that materials and components can be efficiently recovered and reintroduced into material loops after dismantling operations. The integration of DfD principles into SSbD strategies is particularly important because circularity cannot rely solely on material recyclability at the molecular level. Even highly recyclable polymers may fail to achieve circularity if products are assembled in ways that prevent efficient separation or recovery. Therefore, an integrated ecodesign perspective is necessary to align material innovation with downstream waste management and recycling systems.

9.3 Design for recycling

One of the most effective strategies for improving polymer sustainability is **design for recycling**. This approach involves designing materials and products in ways that facilitate their efficient recovery and recycling after use.

One key aspect of design for recycling is **reducing material complexity**. Products composed of multiple polymer types, multilayer structures, or incompatible blends are often difficult to recycle because separating the different materials can be technically challenging and economically costly. Simplifying product designs by using fewer material types can significantly improve recyclability.

Minimizing the use of additives that interfere with recycling processes is another important consideration. Certain pigments, stabilizers, and fillers may alter the physical properties of recycled polymers or contaminate recycling streams. Selecting additives that are compatible with recycling processes helps maintain the quality of recycled materials.

Standardization of polymer materials within specific applications can also improve recycling efficiency. For example, standardized packaging materials enable recycling facilities to sort and process plastic waste more effectively.

9.4 Environmental impacts during use

In addition to durability (9.1), product designers must consider **environmental impacts that occur during the use phase** of polymer products. One increasingly recognized issue is the generation of **microplastics** resulting from the abrasion or fragmentation of polymer materials during use.

Microplastic particles can be generated through various mechanisms, including mechanical wear of polymer surfaces, degradation of synthetic textiles during washing, tire abrasion on road surfaces, and fragmentation of plastic coatings or packaging materials. These particles may accumulate in aquatic and terrestrial environments, potentially affecting ecosystems and food chains.

Design strategies to address this issue include selecting materials that exhibit **high resistance to abrasion**, improving product coatings to reduce surface wear, and developing polymers that degrade into environmentally benign products under specific conditions. For example, certain biodegradable polymers can break down into smaller molecules that are metabolized by microorganisms, reducing long-term environmental persistence.

Another strategy involves designing products with **protective layers or reinforced surfaces** that minimize direct exposure of the polymer to mechanical stress. Improved textile structures and fiber engineering can also reduce fiber shedding during washing, thereby lowering microplastic emissions.

9.5 Smart and functional polymers

Emerging innovations in **smart polymer materials** offer promising opportunities to improve the sustainability of polymer products. Smart polymers are materials that can respond to external stimuli such as temperature, light, mechanical stress, or chemical signals by changing their properties or behavior.

One particularly promising example is the development of **self-healing polymers**. These materials are capable of repairing microcracks or structural damage autonomously through reversible chemical reactions or embedded healing agents. When damage occurs, the polymer network reorganizes or triggers chemical reactions that restore the material's structural integrity.

Self-healing materials have the potential to significantly extend product lifetimes by preventing the propagation of cracks and structural failures. Applications range from coatings and adhesives to structural composites and electronic devices.

Another emerging class of materials includes **recyclable thermosets based on dynamic covalent chemistry**. Conventional thermoset polymers possess permanently crosslinked networks that cannot be melted or reshaped after curing, making them difficult to recycle. Dynamic covalent chemistry introduces reversible bonds within the polymer network, enabling these materials to be reshaped, repaired, or chemically recycled.

These adaptable polymer networks combine the mechanical strength of thermosets with the re-processability typically associated with thermoplastics. As a result, they offer new opportunities to develop durable yet recyclable materials for applications in electronics, automotive components, and advanced composites.

Through the integration of durable materials, advanced polymer architectures, and smart functionalities, product designers can create polymer-based products that meet performance requirements while supporting sustainability goals.

10 Circularity and End-of-Life management

The concept of **circularity** has become a central principle in sustainable materials development and plays a critical role in the SSbD framework. Traditional economic systems have largely followed a **linear model** in which raw materials are extracted, converted into products, and eventually discarded as waste. This approach leads to significant resource depletion, environmental pollution, and inefficient use of valuable materials.

Circular economy principles aim to replace this linear model with systems that prioritize **resource efficiency, material recovery, and waste reduction**. Achieving circularity in polymer systems begins well before a product reaches disposal. As discussed in Section 9.3 (Design for recycling), decisions made during the design stage determine whether a product can realistically be recovered and reprocessed at all. The strategies discussed in this chapter, from recycling technologies to biodegradable alternatives, build directly on those upstream design choices.

Achieving circularity in polymer systems requires careful consideration of both **material design and waste management strategies**. Product designers must anticipate how materials will be collected, sorted, recycled, or recovered after use.

10.1 Recycling technologies

Currently, **mechanical recycling** remains the most widely used method for recovering thermoplastic polymers. In mechanical recycling, plastic waste is collected, sorted, cleaned, and remelted to produce recycled pellets that can be used to manufacture new products.

Mechanical recycling offers several advantages, including relatively low energy consumption and well-established industrial infrastructure. However, repeated recycling cycles may lead to **polymer degradation**, resulting in reduced mechanical properties and material quality. As a result, recycled polymers may be used in lower-value applications through a process known as downcycling.

To complement mechanical recycling, **chemical and biological recycling technologies** are increasingly being developed. Chemical recycling processes break polymer chains into their original monomers or other chemical intermediates that can be

used as feedstocks for new polymer production. Examples include depolymerization, pyrolysis, and gasification processes.

Chemical recycling offers the potential to recover high-purity raw materials from plastic waste, enabling closed-loop recycling systems in which polymers are repeatedly converted into new materials without significant loss of quality.

In addition to chemical recycling, **enzymatic recycling** is emerging as a promising biological route for the selective depolymerization of certain polymers. Enzymatic recycling uses biocatalysts, such as cutinases, PETases, esterases, lipases, or engineered enzymes, to break specific chemical bonds in polymer chains under relatively mild conditions. This technology has received particular attention for **polyethylene terephthalate (PET)**, where enzymes can hydrolyse ester bonds and convert PET into monomers such as terephthalic acid and ethylene glycol, which may subsequently be purified and reused to produce new PET.

Compared with conventional chemical recycling, enzymatic recycling may offer several sustainability advantages, including lower operating temperatures, aqueous reaction media, reduced energy demand, and high selectivity toward target polymer bonds. These characteristics make it especially attractive within a SSbD approach, as it can reduce the use of harsh chemicals and minimize secondary waste streams.

However, enzymatic recycling also presents important technical challenges. Reaction rates can be slow, polymer crystallinity can limit enzyme accessibility, and pre-treatment steps may be required to increase polymer surface area or reduce crystallinity. In addition, enzyme production, stability, reuse, and process scale-up must be optimized to make enzymatic recycling industrially competitive. The technology is therefore especially promising for selected polyester-rich streams, but its broader application will require further advances in enzyme engineering, reactor design, and integration with sorting and pre-treatment systems.

Overall, future circular polymer systems will likely rely on a **portfolio of complementary recycling technologies**. Mechanical recycling will remain essential for clean and well-sorted thermoplastic streams, while chemical and enzymatic recycling can provide additional options for more complex, degraded, or contaminated materials. The selection of the most appropriate recycling pathway should be based on polymer type, waste stream quality, environmental performance, economic feasibility, and compatibility with existing recycling infrastructure.

10.2 Biodegradable and compostable polymers

In some applications, recycling may not be practical due to contamination, product complexity, or dispersed use. In such cases, **biodegradable and compostable polymers** may provide an alternative end-of-life solution.

Polymers and mainly polyesters, such as **polylactic acid (PLA)** and **polyhydroxyalkanoates (PHA)**, can degrade under controlled composting conditions through the action of microorganisms. These materials are often used in applications such as food packaging, agricultural films, and disposable products.

However, the environmental benefits of biodegradable polymers depend strongly on the availability of **appropriate waste management infrastructure**, particularly industrial composting facilities. Without proper composting conditions, biodegradable polymers may persist in the environment similarly to conventional plastics.

10.3 Toward a circular polymer economy

Achieving a truly circular polymer economy will likely require the integration of **multiple complementary strategies**, including improved product design, advanced recycling technologies, biodegradable materials, and effective waste management systems.

In addition, collaboration across the entire value chain - including material producers, product manufacturers, recyclers, policymakers, and consumers - is essential for developing circular systems that maximize resource efficiency and minimize environmental impacts.

By designing polymer materials and products with circularity in mind from the outset, researchers and industry stakeholders can significantly improve the sustainability of polymer systems and support the transition toward a more resource-efficient and environmentally responsible materials economy.

11 Environmental and safety assessment tools

The development of polymer materials that align with the principles of SSbD requires robust methodologies to evaluate their environmental performance and potential impacts on human health and ecosystems. Because polymer materials often involve complex formulations, long life cycles, and diverse applications, it is essential to employ systematic assessment tools that provide quantitative and qualitative information about their sustainability. These tools support informed decision-making during research and development, enabling scientists and engineers to compare alternative materials, identify potential risks, and optimize design strategies.

As introduced in Chapter 2, the SSbD philosophy favours preventing risks over addressing them after commercialization. Environmental and safety assessment tools are what make this possible in practice: they allow for evaluating the environmental burdens and safety issues associated with a polymer material, from raw material extraction and synthesis to manufacturing, use, and end-of-life, early enough in the development process to inform design decisions rather than simply document outcomes after the fact.

Among the most widely used methodologies for evaluating environmental performance is **Life Cycle Assessment (LCA)**. In addition, hazard and toxicity assessments provide insights into potential health and ecological risks associated with chemicals and materials. Complementary metrics such as circularity indicators further support the evaluation of resource efficiency and material recovery potential.

11.1 Life Cycle Assessment

Life Cycle Assessment is a standardized methodology used to evaluate the **environmental impacts of products, materials, and processes across their entire life cycle**. Life cycle perspective is particularly important for polymer materials because environmental impacts may occur at multiple stages, including raw material extraction, polymer synthesis, manufacturing, transportation, product use, and end-of-life management.

The LCA methodology typically follows four main stages: goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and interpretation. During the goal and scope definition phase, the objectives of the study are established, and system boundaries are defined. For example, an LCA study may evaluate the environmental impacts of polymer packaging material from raw material extraction to disposal or recycling.

The **life cycle inventory (LCI)** phase involves collecting detailed data on energy use, material inputs, emissions, and waste generation associated with each stage of the product life cycle. These data are then used in the **life cycle impact assessment (LCIA)** phase to quantify environmental indicators.

LCA can quantify a wide range of environmental impacts, including **greenhouse gas emissions (carbon footprint), cumulative energy demand, water consumption, land use, acidification potential, eutrophication potential, and ozone depletion potential**. These indicators provide valuable insights into how different material choices influence environmental performance.

In polymer research and development, LCA is particularly useful for comparing **bio-based polymers with fossil-based alternatives**, evaluating the benefits of recycling strategies, and identifying opportunities to reduce environmental impacts through improved processing technologies. For example, LCA studies can reveal whether a bio-based polymer actually provides lower greenhouse gas emissions when considering agricultural inputs, transportation, and processing requirements.

By providing a comprehensive evaluation of environmental impacts across the life cycle, LCA supports decision-making processes that aim to minimize the environmental footprint of polymer materials.

11.2 Hazard and toxicity assessment

While environmental impact assessment focuses on resource use and emissions, **hazard and toxicity assessments** are essential for evaluating potential risks to human health and ecosystems. Polymer materials may contain various chemical substances, including monomers, catalysts, additives, stabilizers, and degradation products, each of which may present different toxicological profiles.

Within the SSbD framework, hazard assessment aims to identify and eliminate chemicals that pose unacceptable risks. Early-stage screening of chemical hazards is particularly

important because it allows researchers to substitute problematic substances before they are incorporated into materials or products.

One powerful tool used in hazard screening is the application of **quantitative structure–activity relationship (QSAR) models**. QSAR models use computational methods to predict the biological activity or toxicity of chemical substances based on their molecular structure. These models analyze relationships between chemical structures and observed biological effects, allowing researchers to estimate toxicity without conducting extensive experimental testing.

QSAR approaches are widely used for predicting properties such as **mutagenicity, carcinogenicity, bioaccumulation potential, and aquatic toxicity**. Because QSAR models rely on computational predictions, they can rapidly evaluate large numbers of candidate molecules, making them particularly valuable during early-stage material design.

Although computational methods provide valuable insights, they must often be complemented by **experimental toxicological testing** to confirm predictions and evaluate complex interactions between materials and biological systems. Experimental methods may include **in vitro assays**, which evaluate biological responses in cultured cells, and **ecotoxicity tests**, which assess the effects of chemicals on aquatic organisms such as algae, crustaceans, or fish.

For polymer materials, toxicity assessments may also consider the potential release of **additives, residual monomers, or degradation products** during product use or disposal. Evaluating these potential exposure pathways is critical for ensuring that polymer materials do not pose risks to consumers, workers, or the environment.

Integrating computational predictions with experimental testing provides a comprehensive approach to hazard assessment that supports the development of safer polymer materials.

11.3 Circularity indicators

In addition to environmental impact and toxicity assessments, evaluating the **circularity of materials** is an essential component of sustainable polymer development. Circularity indicators provide quantitative metrics that assess the ability of materials to remain within productive use cycles and minimize waste generation.

One important circularity metric is **recycled content**, which measures the proportion of recycled material incorporated into a product. Increasing recycled content can reduce the demand for virgin raw materials and decrease the environmental impacts associated with resource extraction.

Another key indicator is the **recyclability rate**, which reflects the extent to which a material can be collected, sorted, and processed through existing recycling systems. Materials designed for high recyclability often feature simplified compositions, compatible polymer types, and additives that do not interfere with recycling processes.

Material efficiency is the third important metric that evaluates how effectively raw materials are converted into final products. High material efficiency reduces waste generation during manufacturing and improves overall resource utilization.

Beyond these traditional circularity indicators, increasing attention is being given to concepts related to **Design for Disassembly** and **Design for Deconstruction**- see **Chapter 9.2** - particularly for complex products composed of multiple materials or components.

Other circularity indicators may include product lifetime, repairability, reusability, remanufacturing potential, and recovery efficiency. Products designed with modular architecture and replaceable components may exhibit significantly higher circularity compared with single-use or permanently assembled products. Extending product lifetime through repair and refurbishment can substantially reduce resource consumption and delay waste generation.

In addition, emerging digital technologies such as digital product passports may support circularity evaluation by improving traceability of materials, additives, and recycling information throughout the product life cycle. These tools can facilitate sorting, repair, and end-of-life management by providing detailed information on material composition and dismantling procedures.

By combining circularity indicators with environmental impact assessments, hazard evaluations, and design-for-disassembly principles, researchers and industrial stakeholders can evaluate polymer materials from a comprehensive systems perspective. This integrated approach enables the development of products that are not only safe and sustainable during production and use, but also optimized for efficient recovery, reuse, and reintegration into circular material flows at the end of their life cycle.

By combining circularity indicators with environmental and safety assessments, researchers can evaluate polymer materials from a **systems perspective**, considering not only their environmental impacts but also their potential to support circular material flows.

11.4 Integrating assessment tools into SSbD

The integration of LCA, hazard evaluation, and circularity indicators provides a comprehensive framework for evaluating the sustainability of polymer materials. These tools allow researchers and industry stakeholders to identify trade-offs between different design choices and select materials that offer the best balance between performance, safety, and environmental sustainability.

Importantly, as noted at the beginning of this chapter, assessment tools should not be applied only at the final stages of product development. Instead, they should be incorporated into the **early phases of material design**, where they can guide the selection of monomers, additives, processing methods, and product architectures.

By embedding environmental and safety assessment tools within the SSbD framework, polymer researchers can develop materials that not only meet technical performance requirements but also contribute to a safer and more sustainable materials economy.

12 Digital tools for SSbD polymer innovation

The rapid advancement of digital technologies is fundamentally transforming the way polymer materials are discovered, designed, and optimized. Traditionally, polymer development has relied heavily on experimental trial-and-error approaches, which can be time-consuming, resource-intensive, and costly. Researchers often needed to synthesize and characterize large numbers of polymer formulations before identifying materials that met the desired performance and safety requirements. Within the SSbD framework, such conventional development approaches are increasingly being complemented - and in some cases replaced - by **digital tools that enable predictive design and data-driven decision-making**.

Digital technologies allow researchers to explore a wide range of potential polymer structures and compositions before laboratory synthesis begins. By predicting material properties, environmental impacts, and safety profiles early in the development process, these tools significantly accelerate innovation while reducing material consumption, experimental waste, and research costs. As a result, digitalization plays a crucial role in enabling the efficient development of polymer systems that meet both **performance requirements and sustainability objectives**.

Among the most important digital approaches used in polymer innovation are **computational chemistry, molecular modeling, machine learning, and integrated data platforms**. Together, these tools provide powerful capabilities for predicting polymer properties, screening candidate materials, and supporting sustainability assessments.

12.1 Computational modeling and molecular simulation

Computational modeling techniques are increasingly used to simulate polymer structures and predict their physical and chemical properties. These methods rely on mathematical models and numerical simulations to describe the behavior of polymer molecules at different scales, ranging from the atomic level to macroscopic material properties.

One common approach is **molecular dynamics (MD) simulation**, which models the movement and interactions of atoms and molecules over time. Molecular dynamics simulations allow researchers to analyze polymer chain conformations, intermolecular interactions, and structural dynamics under different conditions. These simulations provide valuable insights into how polymer architecture influences material properties such as mechanical strength, flexibility, and thermal stability.

Another widely used computational approach is **quantum chemical modeling**, which can be used to investigate the electronic structure of polymer building blocks and

chemical reactions involved in polymer synthesis. Quantum mechanical calculations help researchers understand reaction mechanisms, predict polymerization pathways, and design monomers with improved reactivity or stability.

At larger scales, **coarse-grained modeling** techniques simplify complex polymer systems by grouping atoms into larger units, allowing simulations of larger systems over longer time scales. These models are particularly useful for studying polymer morphology, phase behavior, and interactions in polymer blends and composites.

Computational modeling can also be used to predict important polymer properties such as **glass transition temperature (T_g), melting temperature, mechanical modulus, permeability, and chemical stability**. Predicting these properties before synthesis enables researchers to evaluate a large number of potential polymer structures and identify promising candidates for experimental validation.

This predictive capability is particularly valuable in the development of sustainable polymers because it allows researchers to evaluate **bio-based monomers, degradable polymer architectures, and recyclable materials** without extensive experimental testing.

12.2 Machine learning and artificial intelligence

While computational chemistry provides detailed insights into molecular behavior, **machine learning (ML) and artificial intelligence (AI)** offer powerful tools for analyzing large datasets of polymer properties and identifying patterns that can guide materials discovery.

Machine learning algorithms can be trained using datasets containing information on polymer structures, synthesis conditions, and measured properties. Once trained, these models can predict the properties of new polymer candidates based on their chemical structure or formulation.

For example, machine learning models can predict properties such as **glass transition temperature, tensile strength, degradation behavior, and barrier performance** based on structural descriptors of polymer chains. This capability allows researchers to rapidly screen thousands of potential polymer structures and focus experimental efforts on the most promising candidates.

Machine learning is also increasingly used to design **polymer formulations and additives** that optimize specific performance characteristics. By analyzing complex relationships between polymer composition, processing conditions, and material performance, machine learning algorithms can identify combinations that might not be immediately obvious through traditional experimental approaches.

In addition to property prediction, AI methods are being used to **optimize polymer synthesis and processing conditions**. AI-driven optimization algorithms can analyze experimental data to identify optimal temperature profiles, catalyst concentrations, or processing parameters that maximize material performance while minimizing energy consumption or waste generation.

These capabilities significantly accelerate the development of new polymer materials and contribute to more efficient and sustainable innovation processes.

12.3 Digital platforms for sustainability assessment

Beyond materials discovery, digital tools also play an increasingly important role in supporting **sustainability assessment and decision-making**. Integrated digital platforms can combine data from multiple sources - including LCA, hazard databases, regulatory information, and performance metrics - to evaluate the overall sustainability profile of polymer materials.

Such platforms allow researchers and product developers to assess trade-offs between different design choices. For example, a polymer with excellent mechanical properties may require energy-intensive synthesis, while an alternative polymer may offer lower environmental impacts but slightly reduced performance. Digital decision-support systems can help identify optimal solutions that balance functionality with environmental and safety considerations.

Digital sustainability platforms often incorporate **databases containing environmental impact factors, toxicity data, and regulatory classifications**. By linking this data with material design tools, developers can screen candidate materials against sustainability criteria early in the development process.

For instance, integrated SSbD platforms may evaluate whether a proposed polymer formulation contains substances of very high concern (SVHC), estimate its life cycle carbon footprint, and assess its compatibility with existing recycling systems. This information enables developers to refine material designs before investing in experimental validation or industrial scale-up.

12.4 Digital twins and smart manufacturing

Another emerging application of digital technologies in polymer innovation involves the use of **digital twins** and smart manufacturing systems. A digital twin is a virtual representation of a physical manufacturing process that continuously receives data from sensors and monitoring systems.

By simulating polymer processing operations in real time, digital twins allow manufacturers to optimize production conditions, predict equipment performance, and reduce energy consumption. For example, digital models of extrusion processes can help identify optimal temperature profiles, screw speeds, and material feed rates that improve process efficiency while maintaining product quality.

Smart manufacturing technologies also enable predictive maintenance, reducing equipment downtime and minimizing energy losses associated with inefficient operations.

12.5 Accelerating SSbD implementation through digitalization

The integration of computational modeling, machine learning, and digital decision-support systems provides a powerful toolkit for implementing the SSbD framework in polymer research and development. These technologies allow researchers to evaluate safety, environmental performance, and material functionality simultaneously during the design phase.

By reducing the reliance on trial-and-error experimentation, digital tools accelerate innovation while lowering material consumption and laboratory waste. This approach aligns closely with the goals of sustainable materials development by improving resource efficiency and enabling more informed design decisions.

As computational power continues to increase and data availability expands, digital technologies are expected to play an increasingly central role in polymer science. The combination of **advanced modeling techniques, artificial intelligence, and integrated sustainability platforms** will enable the rapid development of polymer materials that meet the complex requirements of safety, performance, and environmental sustainability.

Ultimately, digital tools are transforming polymer innovation from an experimental trial-and-error process into a **predictive, data-driven discipline**, enabling the efficient design of next-generation materials that support a safe and sustainable materials economy.

13 SSbD innovation workflow for polymer development

The successful implementation of the SSbD framework requires structured innovation processes that integrate sustainability, safety, and performance considerations throughout the entire development pathway. Polymer innovation typically involves complex research and development activities, ranging from molecular design and laboratory synthesis to industrial manufacturing and product commercialization. Without a systematic workflow, sustainability assessments may be introduced too late in the process, when material choices and design parameters are already fixed.

To address this challenge, structured innovation frameworks such as the **stage-gate model** are increasingly used to guide polymer development. The stage-gate approach divides the innovation process into a sequence of development stages separated by decision points, or “gates.” At each gate, predefined criteria are evaluated to determine whether the project should proceed to the next stage, be modified, or be terminated. Integrating SSbD principles into this model ensures that safety and sustainability considerations are incorporated alongside technical performance from the earliest stages of development.

The SSbD innovation workflow for polymer development typically consists of five main stages: **concept definition, design, development, validation, and scale-up**. Each stage includes specific technical activities as well as environmental and safety evaluations that support responsible material innovation.

13.1 Concept definition and sustainability objectives

The first stage of the SSbD workflow focuses on **defining the intended function of the polymer material and establishing sustainability objectives**. At this early stage, researchers identify the application area of the material, such as packaging, automotive components, electronics, medical devices, or construction materials. The functional requirements of the polymer - such as mechanical strength, thermal stability, barrier properties, flexibility, or chemical resistance - are clearly defined.

At the same time, sustainability objectives are established in alignment with SSbD principles. These objectives may include reducing greenhouse gas emissions, increasing the use of renewable feedstocks, minimizing hazardous substances, improving recyclability, or reducing energy consumption during manufacturing. Defining sustainability targets early in the development process ensures that environmental considerations are integrated into the material design rather than addressed as an afterthought.

During this stage, researchers also evaluate **regulatory requirements and market expectations**. Environmental regulations, safety standards, and consumer preferences increasingly influence material selection and product development. Understanding these external drivers helps guide the development of polymer materials that meet both regulatory compliance and market demands.

The concept stage concludes with an initial feasibility assessment that evaluates the technical and environmental potential of the proposed material concept.

13.2 Material design and candidate selection

Once the functional requirements and sustainability objectives have been established, the next stage focuses on **material design and the selection of candidate polymer systems**. During this phase, researchers identify potential monomers (**Chapter 5**), polymer architecture (**Chapter 5**), synthesis pathways (**Chapter 6**), and additives (**Chapter 7**) that can deliver the desired properties.

Material design decisions are informed by both **performance considerations and safety assessments**. Computational modeling tools, molecular simulations, and machine learning algorithms may be used to predict polymer properties and identify promising candidate materials. These digital tools can accelerate the screening of large numbers of potential polymer structures, reducing the need for extensive experimental testing.

Hazard screening is also conducted at this stage to ensure that selected monomers and additives do not present unacceptable risks. Databases containing information on

toxicological properties and regulatory classifications can help identify substances of concern and guide the selection of safer alternatives.

In addition to safety considerations, material design also incorporates **circularity principles**. Researchers evaluate whether candidate polymer structures are compatible with existing recycling technologies, whether they contain degradable linkages that facilitate chemical recycling, and whether additives may interfere with recycling processes.

The design stage typically concludes with the selection of one or more candidate polymer systems that satisfy both technical performance requirements and preliminary sustainability criteria.

13.3 Development and prototype testing

The **development stage** involves synthesizing and characterizing prototype polymer materials in the laboratory. At this stage, experimental work focuses on verifying the predicted properties of candidate materials and optimizing synthesis conditions.

Researchers conduct a wide range of **material characterization tests**, including measurements of mechanical properties, thermal behavior, chemical resistance, and durability. These tests provide valuable insights into how polymer structure influences performance and help identify potential improvements in material formulation.

In parallel with performance testing, **safety assessments** are conducted to evaluate potential risks associated with the polymer system. These assessments may include the evaluation of residual monomers, additive migration, and degradation products that could be released during product use or disposal.

Environmental considerations are also addressed during the development stage. **Preliminary LCA** may be conducted to estimate the environmental impacts associated with raw material production, polymer synthesis, and processing. These assessments help identify opportunities to reduce energy consumption, minimize waste generation, and improve resource efficiency.

The development stage is highly iterative, with researchers refining polymer formulations and synthesis methods based on experimental results and sustainability evaluations.

13.4 Validation and sustainability assessment

Once prototype materials have been successfully developed, the next stage focuses on **validation and a comprehensive sustainability assessment**. The goal of this stage is to evaluate whether the polymer material meets predefined performance, safety, and sustainability criteria.

A key component of validation is the application of **LCA** to quantify the environmental impacts associated with the material. LCA studies evaluate indicators such as greenhouse

gas emissions, energy consumption, water use, and resource depletion across the entire life cycle of the product.

Hazard evaluations are also conducted to confirm that the material does not contain substances of concern or pose unacceptable risks to human health or ecosystems. These evaluations may involve both computational toxicity predictions and experimental testing methods.

Circularity assessments are another important aspect of validation. Researchers evaluate the recyclability of the polymer material, its compatibility with existing recycling infrastructure, and the potential for reuse or repair of products made from the material.

The validation stage ensures that the material aligns with SSbD principles and provides a robust evidence base for decision-making before moving to industrial-scale production.

13.5 Scale-up and industrial implementation

The final stage of the SSbD innovation workflow involves **scaling up the production process and preparing the material for industrial implementation**. Laboratory-scale synthesis methods must be adapted for large-scale manufacturing while maintaining product quality, safety, and sustainability performance.

Process optimization plays a critical role during scale-up. Engineers evaluate processing parameters such as temperature, pressure, catalyst concentration, and reaction time to ensure efficient and reliable production. Energy consumption, waste generation, and resource efficiency are carefully monitored to minimize environmental impacts.

Industrial implementation also requires compliance with regulatory standards related to chemical safety, environmental protection, and product performance. Certification and testing procedures may be required before polymer products can be introduced to the market.

At this stage, collaboration between research institutions, industrial partners, and regulatory authorities becomes essential. Technology transfer activities ensure that laboratory innovations can be successfully translated into commercial products.

13.6 Integrating sustainability throughout the innovation process

The SSbD innovation workflow emphasizes the importance of **continuous evaluation and iterative improvement**. Sustainability and safety assessments are not confined to a single stage but are integrated throughout the entire development process.

By applying structured innovation frameworks such as the stage-gate model (**Figure 4**), organizations can ensure that polymer materials are developed in a way that balances functionality, safety, environmental sustainability, and circularity. This approach reduces the risk of costly redesigns, improves regulatory compliance, and accelerates the

development of materials that support a more sustainable and responsible polymer industry.

Ultimately, the integration of SSbD principles into polymer innovation workflows represents a critical step toward creating materials that meet the complex technological and environmental challenges of the future.

SSbD Decision Tree for Polymer Design

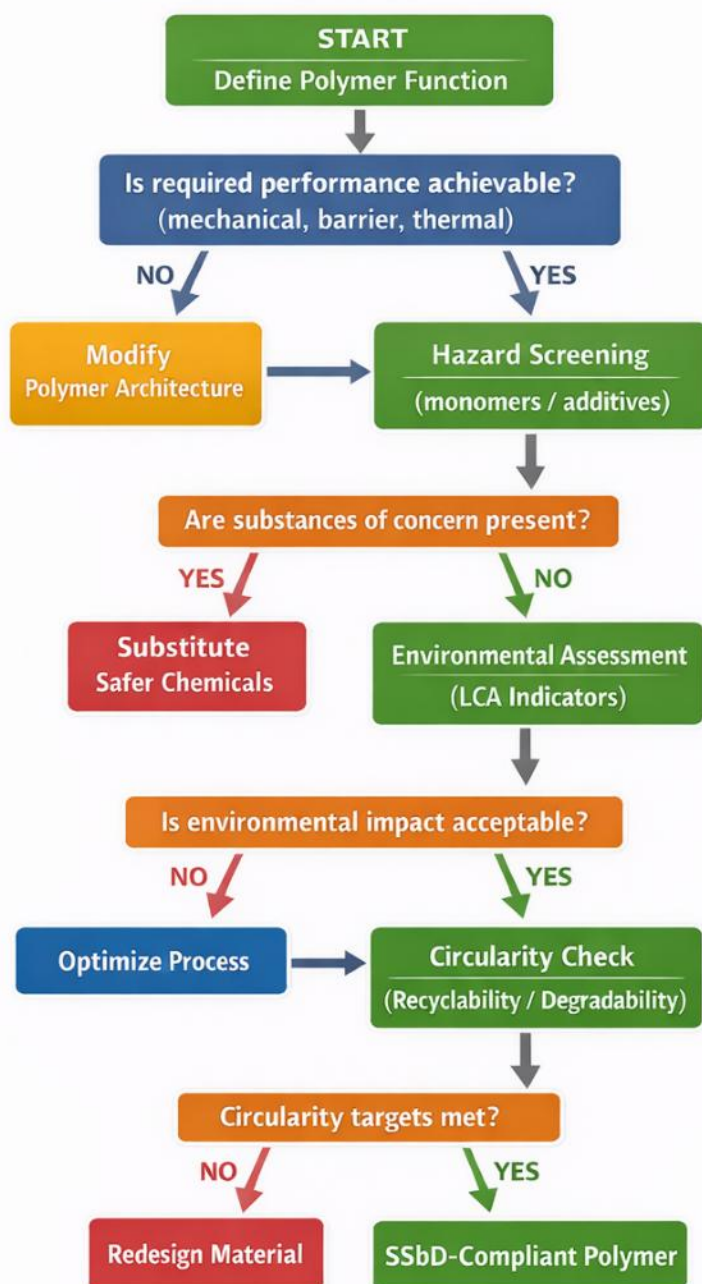


Figure 4. SSbD decision tree for polymer design (outcome of the project)

14 Main challenges identified for SSbD implementation

Despite the significant opportunities offered by the SSbD framework, the implementation of this approach in the development of polymeric materials faces several important challenges.

Within the framework of the *Knowledge Book on Best Practices: SSbD Polymer and Product Development*, the main challenges associated with the implementation of the SSbD approach were systematically identified. This analysis was based on the expertise and practical experience of the project's technical partners. Through a structured questionnaire, each partner assessed the challenges encountered from the perspective of its specific role and responsibilities within the project, providing insights across the different stages of polymer and product development, testing, scale-up and validation. The consolidated results offer a comprehensive overview of these challenges, which can be broadly categorized into **general systemic challenges** and **specific technical challenges related to polymer development and industrial implementation**.

(More detailed information on the analysis is available in the **ANNEX**).

14.1 General systemic challenges

One of the most critical challenges concerns the **substitution of substances of concern while maintaining material functionality**. Many polymer formulations currently rely on additives and processing aids that have well-established performance characteristics but may pose environmental or health risks. Identifying safer alternatives that deliver equivalent technical performance requires extensive research into the chemical, toxicological, and physical properties of candidate substances. In addition, the environmental impacts of alternative substances must be evaluated across their entire life cycle to ensure that substitution does not inadvertently introduce new sustainability problems.

Another major challenge relates to the **implementation of life cycle thinking in material development**. Although methodologies such as Life Cycle Assessment, Carbon Footprint analysis, and Water Footprint analysis are increasingly recognized as essential tools for sustainability evaluation, their systematic application within industrial R&D processes remains limited. Many companies still lack the data, expertise, or modeling capabilities required to perform these assessments during early development stages. Furthermore, applying LCA to emerging materials requires complex process modeling and scenario development, which introduces additional uncertainties.

The development of **innovative technologies for sustainable polymer production** also presents important technical and economic challenges. Creating new materials and production processes that meet SSbD standards often requires significant investments in research infrastructure, pilot-scale facilities, and multidisciplinary expertise. At the same time, regulatory frameworks governing chemical safety and environmental protection are

continuously evolving, creating uncertainty for long-term research and development strategies.

Access to reliable data and effective collaboration among stakeholders represent additional challenges. Implementing SSbD principles requires the integration of information from multiple sources, including chemical hazard databases, environmental impact assessments, and industrial process data. Ensuring that these data are accessible, interoperable, and reusable in accordance with FAIR data principles is essential for supporting evidence-based decision-making. Collaboration between industry, academia, research centers, and regulatory authorities is therefore crucial for advancing the development of sustainable polymer systems.

Education and capacity building also play a key role in the successful implementation of SSbD strategies. Polymer scientists, engineers, and product designers must develop expertise not only in materials science but also in sustainability assessment, toxicology, and circular economy principles. Updating educational curricula and professional training programs to include SSbD concepts will be essential for preparing the next generation of materials researchers and industrial practitioners.

Regulatory alignment represents another important challenge. The development of sustainable polymer materials must comply with a complex and evolving regulatory landscape, including regulations related to chemical safety, packaging waste, occupational exposure, and environmental protection. For example, new regulatory developments addressing reprotoxic substances, microplastics, and PFAS compounds require material developers to anticipate potential restrictions and adapt their design strategies accordingly.

Economic considerations also influence the adoption of sustainable materials. Although environmentally friendly materials may provide long-term benefits in terms of resource efficiency and reduced environmental impacts, their production costs can be higher than those of conventional materials. Achieving economic competitiveness requires technological innovation, supportive policy frameworks, and market incentives that encourage the adoption of sustainable materials.

14.2 Technical challenges in polymer Development

Beyond these systemic challenges, several **specific technical challenges** have been identified in relation to polymer materials and their industrial implementation.

One of the most significant technical issues concerns the **processability of recycled polymers**. Recycled materials often exhibit degraded properties that affect their processing behavior during extrusion, injection molding, or compounding operations. To restore processability and mechanical performance, additives such as stabilizers, fillers, coupling agents, and processing aids are frequently required. However, balancing the need for such additives with SSbD requirements, particularly the avoidance of hazardous substances, represents a complex formulation challenge.

Another critical issue is the growing concern regarding **microplastics and their environmental impacts**. Polymer materials can generate microplastic particles during product use or degradation, raising concerns about their environmental persistence and associated ecological risks. Addressing this challenge requires the development of materials that minimize particle release or degrade into environmentally benign substances under controlled conditions.

Recyclability also depends heavily on **the effectiveness of material sorting technologies**. Optical sorting systems based on near-infrared (NIR) spectroscopy are widely used to identify polymer types in recycling facilities. However, certain pigments, fillers, or multilayer structures may interfere with NIR detection, reducing the efficiency of sorting processes. Designing materials that are compatible with existing sorting technologies is therefore an important aspect of circular polymer design.

The **market dynamics of recycled polymer raw materials** also present challenges. Fluctuations in the price of virgin petrochemical feedstocks can significantly influence the economic competitiveness of recycled polymers. When virgin materials become cheaper, demand for recycled polymers may decline, affecting the viability of recycling infrastructure and investment in new recycling technologies such as chemical recycling.

Another technical barrier relates to **scaling up new sustainable materials from laboratory to industrial production**. Processes that perform well at laboratory scale may encounter difficulties when implemented at larger scales due to changes in reaction kinetics, heat transfer, mixing efficiency, or raw material availability. Ensuring consistent material quality during scale-up requires careful process engineering and optimization.

Finally, the **control of toxicity and ecotoxicity throughout the material life cycle** represents an ongoing challenge. New regulatory frameworks addressing reprotoxic substances and occupational exposure limits require developers to evaluate potential risks associated with polymer synthesis, processing, and product use. This includes monitoring potential impurities, degradation products, and emissions that may arise during manufacturing or product use.

14.3 REPurpose project specific challenges

Beyond the general and technical challenges common to SSbD implementation in the polymer sector, the REPurpose project encountered challenges tied to its own materials, technologies, and consortium structure. These fall into three main areas: assessing costs and environmental impacts under high technological uncertainty, analytical and experimental constraints affecting execution, and coordinating material development with downstream prototyping and testing.

Benchmarking costs and environmental impacts was made difficult by the novelty of the molecules and processes involved, which offered little industrial reference data to build on and required both technical and sustainability experts to work closely together under considerable uncertainty.

Analytical and experimental constraints, from unexpected measurement difficulties to limited benchmark materials and small sample sizes in early development, slowed decision-making and underlined the importance of flexible planning and early involvement of downstream partners.

Align material development with product design, prototyping, and testing proved organizationally demanding, as the iterative nature of the work and occasional supply or specification issues repeatedly required adjustments across the consortium.

14.3.1 Challenges for industrial uptake

Beyond project execution, partners also identified structural barriers that may affect the transferability and industrial uptake of the proposed Best Practices, spanning scale-up engineering, market and regulatory conditions, and the durability of impact beyond the project itself. Full details are provided in the Annex.

Moving from pilot to industrial scale raises some challenges, from maintaining consistent material quality at larger volumes to managing by-product removal and process productivity, meaning plant design will need to be specifically adapted to REP materials rather than simply scaled up.

Market uptake is equally uncertain: bio-based and circular materials tend to cost more than fossil-based alternatives, and their competitiveness depends on factors largely outside the consortium's control, such as policy incentives and the stability of recycled raw material prices.

The regulatory landscape adds a further layer of uncertainty, as evolving requirements around substances of concern and product-level sustainability mean companies must anticipate change rather than design for today's rules alone.

For some applications, particularly those involving biodegradability, there is also a genuine tension between guaranteeing performance during use and ensuring materials are credibly and practically compatible with existing waste management and sorting systems.

Finally, sustaining the project's impact once it ends is itself a challenge, requiring continued dissemination and stakeholder engagement through mechanisms such as sectoral alliances or standardization efforts that outlast the project's own timeline.

15 Solutions to simplify SSbD implementation in polymer development

Having identified the general, technical, project-specific, and future-implementation challenges associated with SSbD in polymer development, this chapter presents the corresponding solutions developed and applied within REPurpose. Each of the three sections below responds directly to the challenge group of the same name in **Chapter 14**.

15.1 Solutions to general challenges

Addressing the general challenges of SSbD implementation requires a systemic, forward-looking approach that brings regulatory compliance, sustainability assessment, and innovation management together from the earliest stages of development, rather than treating them as separate workstreams. Many of the barriers identified by the REPurpose partners - including uncertainty regarding future regulatory compliance, difficulties in substituting hazardous substances, limited availability of sustainability data, and costly redesigns during scale-up - stem from decisions being taken independently, by different disciplines, at different stages of the innovation cycle.

The starting point is therefore to integrate safety, sustainability, functionality and circularity into decision-making from the outset, rather than evaluating them sequentially or only at the end of development. When these dimensions are treated as complementary design criteria that evolve together as new experimental evidence becomes available, potential trade-offs surface earlier, reducing the likelihood of selecting development pathways that later prove technically, environmentally or economically unsuitable. Within REPurpose, this was supported through continuous interaction between polymer developers, sustainability experts, toxicologists, process engineers and industrial partners: combining experimental results with prospective sustainability assessments, regulatory monitoring and industrial feedback allowed iterative optimisation of materials before critical scale-up decisions were taken. This translated into concrete outputs (an inventory and roadmap of hazardous additives, and this Best Practice Guide itself ²⁷) intended to help other developers apply the same approach.

Techno-economic and environmental uncertainties were addressed by treating TEA and prospective LCA not as a final validation step, but as tools used iteratively throughout development. Best practice consists of scenario-based modelling with sensitivity analyses to manage uncertainty, boundary conditions aligned with realistic industrial productivity assumptions, and updating TEA/LCA models in parallel with laboratory and pilot-scale data as it becomes available²⁸⁻²⁹.

This integrated modeling approach enables early identification of productivity bottlenecks (e.g., long residence times in depolymerization, high dilution factors) and supports process intensification strategies before large-scale capital investment³⁰.

Finally, given the rapid evolution of European legislation (e.g., Directive (EU) 2022/431 on reprotoxic substances, REACH updates, PPWR), REPurpose set up structured regulatory intelligence systems: continuous monitoring of ECHA and European

²⁷ <https://www.repurposeproject.eu/en/project-outcomes/>

²⁸ Langkau, S., Steubing, B., Mutel, C., Ajie, M. P., Erdmann, L., Voglhuber-Slavinsky, A., & Janssen, M. (2023). A stepwise approach for Scenario-based Inventory Modelling for Prospective LCA (SIMPL). *The International Journal of Life Cycle Assessment*, 28(9), 1169-1193.

²⁹ Wender, B. A., Foley, R. W., Hottle, T. A., Sadowski, J., Prado-Lopez, V., Eisenberg, D. A., ... Seager, T. P. (2014). Anticipatory life-cycle assessment for responsible research and innovation. *Journal of Responsible Innovation*, 1(2), 200–207. <https://doi.org/10.1080/23299460.2014.920121>

³⁰ Arvidsson, R., Tillman, A. M., Sandén, B. A., Janssen, M., Nordelöf, A., Kushnir, D., & Molander, S. (2018). Environmental assessment of emerging technologies: recommendations for prospective LCA. *Journal of Industrial Ecology*, 22(6), 1286-1294.

Commission updates, early hazard classification screening of new monomers, additives, and degradation products and integration of occupational exposure assessments into process development. ECHA provides guidance on carcinogens, mutagens and reprotoxic substances³¹.

Embedding regulatory foresight into R&D governance structures prevents late-stage compliance disruptions and ensures long-term material viability across MS.

15.2 Solutions to specific technical challenges

The technical challenges linked to polymer processability, recyclability, and scale-up called for solutions rooted in materials and process engineering.

On **formulation**, balancing processability with SSbD requirements meant favouring multifunctional additives that reduce formulation complexity, reactive compatibilization to improve recycled polymer performance without excessive stabilizer loading, and a gradual shift toward inherently safer, bio-based alternatives, supported by digital screening tools to accelerate compatibility testing. Digital formulation tools and high-throughput screening platforms helped accelerate additive compatibility testing while minimising the number of hazardous candidates that needed to be screened experimentally. Digital formulation tools and high-throughput screening platforms helped accelerate additive compatibility testing while minimising the number of hazardous candidates that needed to be screened experimentally.

To address **recyclability and NIR detectability challenges**, material design should incorporate optical signature validation during formulation development. Furthermore, avoidance of pigments and fillers that interfere with NIR sorting, and early collaboration with recyclers and sorting technology providers is highly recommended.

The Ellen MacArthur Foundation provides practical guidance on design for recyclability in plastics³².

Integrating recyclability testing into the development stages helps reduce downstream incompatibilities with mechanical recycling streams. Applying protocols such as Recyclclass³³ and considering their guidelines early in the process enables ecodesign to become a key driver and requirement in material development.

Scale-up challenges, from by-product removal to maintaining molecular weight consistency at larger volumes, were addressed through modular pilot-scale validation ahead of full industrial deployment, process intensification techniques such as reactive extrusion and continuous-flow reactors, and in-line Process Analytical Technology (PAT) to keep material quality and productivity under control as production scales up.

³¹ <https://echa.europa.eu/regulations/clp/understanding-clp>

³² <https://ellenmacarthurfoundation.org/the-new-plastics-economy>

³³ <https://recyclclass.eu/>

The European Process Intensification Roadmap³⁴ (SPIRE initiative) provides relevant industrial examples. By integrating scalable engineering criteria early in development, TRL transitions become technically and economically smoother.

15.3 Solutions to REPurpose project specific challenges

The challenges that emerged from REPurpose's own materials and consortium structure called for solutions centered on communication and coordination, more than on any single technology.

Keeping material development aligned with prototyping and testing required a more structured, gated way of working: defined technical-readiness checkpoints before materials were handed off to downstream partners, pre-agreed material specification windows (e.g., acceptable molecular weight range, viscosity tolerance), and, wherever feasible, parallel rather than sequential testing. Agile-inspired coordination - short technical sprints, rapid feedback loops, structured change management - made the consortium more responsive when working with experimental, evolving materials.

Uncertainty in cost and environmental modelling was reduced through closer, more continuous dialogue between experimental developers and sustainability modellers: regular synchronisation between laboratory teams and TEA/LCA analysts, transparent documentation of underlying assumptions, and early agreement on realistic "minimum viable" industrial scenarios rather than extrapolating too far from limited data. This bidirectional feedback loop kept experimental progress and modelled industrial projections consistent with each other, and supported solutions that balanced technical, functional and sustainability considerations together.

The analytical bottlenecks and small early-stage sample sizes that slowed decision-making were managed by building flexibility into experimental planning and involving downstream testing and end-of-life partners earlier, so that limited data could still inform meaningful decisions.

Finally, to ensure continuity beyond the project's own lifetime, REPurpose pursued engagement with standardisation bodies (CEN, ISO) to translate project results into technical standards, industrial clustering and cross-sector alliances to support future scale-up investment, and the development of exploitation roadmaps including IP strategy and licensing frameworks.

The Horizon Europe exploitation guidance provides practical tools for this transition³⁵.

Sustained stakeholder engagement ensures that technical innovation translates into real industrial transformation.

³⁴ <https://www.spire2030.eu>

³⁵ https://rea.ec.europa.eu/dissemination-and-exploitation_en

15.4 Concluding perspective

Overcoming the challenges identified across the previous chapter requires an integrated innovation ecosystem approach, isolated technical fixes are not enough. Successful implementation depends on aligning molecular design, toxicological safety, regulatory foresight, process scalability, sustainability modelling, and market economics at the same time. The REPurpose project showed that embedding SSbD principles, iterative sustainability assessment, proactive regulatory compliance, and structured cross-disciplinary coordination together provide a replicable framework for accelerating the transition toward circular, safe, and economically viable polymeric materials.

16 Best practice guideline and final conclusions

In conclusion, the development of polymeric materials under the SSbD framework requires a holistic and multidisciplinary approach that integrates material science, toxicology, environmental assessment, regulatory compliance, and industrial process engineering. Based on the analysis presented throughout this handbook, several key best practice guidelines can be identified to support the successful implementation of SSbD principles in polymer innovation.

The transition toward safer and more sustainable polymeric materials represents one of the most significant transformations currently taking place within the chemical and materials industries. Throughout this handbook, the SSbD framework has been presented as a comprehensive strategy to guide polymer innovation in a way that integrates functionality, safety, environmental sustainability, and circularity from the earliest stages of development.

The different sections of this document have explored the multiple dimensions involved in the development of SSbD polymer systems. Beginning with the conceptual foundations of SSbD, the handbook highlighted the importance of integrating sustainability and safety considerations into material innovation rather than addressing environmental and safety issues only after materials have been developed and commercialized. The SSbD approach requires a shift from reactive to proactive design strategies, in which potential environmental and health risks are anticipated and minimized during the molecular design phase.

The discussion on **polymer design for safety and sustainability** emphasized the central role of monomer selection, polymer architecture, and molecular functionality in determining the environmental performance of polymer materials. The incorporation of bio-based building blocks, degradable linkages, and dynamic polymer networks illustrates the opportunities available to develop materials that combine high performance with improved sustainability characteristics. At the same time, careful control of additives and polymer formulations is essential to avoid hazardous substances and prevent the release of harmful compounds during product use or disposal.

Sustainable **polymer synthesis and processing technologies** were also identified as critical components of SSbD implementation. Green polymerization methods, solvent-free processes, reactive extrusion, and energy-efficient manufacturing technologies can significantly reduce the environmental footprint associated with polymer production. In addition, innovations in catalyst design, process intensification, and digital monitoring technologies contribute to improved efficiency and lower emissions across industrial processes.

The handbook also highlighted the importance of **product design strategies** that support sustainability throughout the entire life cycle of polymer materials. Designing for durability, reparability, and recyclability ensures that polymer products remain in productive use for longer periods and reduce the generation of waste. Emerging technologies such as self-healing polymers and recyclable thermosets further expand the range of sustainable material solutions available for advanced applications.

Circular economy principles were identified as a key pillar of SSbD polymer innovation. Designing materials that can be effectively recycled, reused, or recovered at the end of their life is essential for reducing dependence on virgin resources and minimizing environmental impacts. Mechanical recycling, chemical recycling, and biodegradable polymer systems represent complementary strategies that can contribute to a more circular polymer economy.

The integration of **environmental and safety assessment tools**, including Life Cycle Assessment (LCA), hazard screening, and circularity indicators, provides the analytical foundation for evaluating the sustainability performance of polymer materials. These tools enable researchers and industry stakeholders to quantify environmental impacts, identify potential risks, and compare alternative material solutions.

In addition, the increasing availability of **digital tools for polymer innovation**, including computational modeling, machine learning, and data-driven design platforms, offers powerful opportunities to accelerate the development of sustainable materials. These technologies enable researchers to predict polymer properties, optimize formulations, and assess environmental impacts before experimental synthesis takes place.

Finally, the **SSbD innovation workflow for polymer development** demonstrated the importance of structured development processes that integrate sustainability assessment, safety evaluation, and technical performance testing across all stages of the material innovation process. By applying stage-gate approaches and iterative evaluation frameworks, organizations can ensure that sustainability objectives are consistently addressed throughout research, development, and industrial scale-up activities.

16.1 Recommendations

The implementation of the SSbD framework and the development of new polymers face several systemic and technical challenges, as extensively discussed in Chapter 14 (e.g., the substitution of hazardous substances, LCA integration, scalability, and market dynamics). Based on the solutions proposed in Chapter 15, the following eight operational recommendations summarize best practices for overcoming these obstacles (**Figure 5**):

16.1.1 Integrate sustainability at the earliest stages of material design

One of the most critical principles of SSbD implementation is the **early integration of sustainability and safety considerations into the material design process**. Rather than addressing environmental impacts and toxicological concerns after materials have been developed, these factors should be considered during the earliest stages of molecular design.

Material developers should evaluate the safety profiles of monomers, catalysts, and additives before synthesis begins. Preference should be given to substances that exhibit low toxicity, low environmental persistence, and minimal potential for bioaccumulation. Whenever possible, **bio-based building blocks and renewable feedstocks** should be considered as alternatives to fossil-based materials, provided that they offer comparable technical performance and do not introduce unintended environmental trade-offs.

Early hazard screening tools, predictive toxicology models, and regulatory databases can support the identification of safer chemical alternatives. This proactive approach reduces the risk of late-stage reformulation and helps ensure long-term regulatory compliance.

16.1.2 Apply life cycle thinking throughout the development process

A second key guideline is the systematic application of **life cycle thinking** in the design and evaluation of polymer materials. Sustainability assessments should not focus solely on the production stage but must consider environmental impacts across the entire life cycle of the material, including raw material extraction, manufacturing, product use, and end-of-life management.

Life Cycle Assessment (LCA), carbon footprint analysis, and water footprint analysis provide valuable tools for evaluating environmental performance and identifying opportunities for improvement. However, these assessments should be applied iteratively throughout the development process, particularly when new materials or processing technologies are being introduced.

The integration of **prospective LCA and techno-economic assessment (TEA)** is especially important when developing innovative materials or processes that have not yet reached industrial scale. Scenario-based modeling and sensitivity analysis can help manage uncertainties and guide decision-making during early research stages.

16.1.3 Design polymer systems for circularity

Circular economy principles must play a central role in the design of new polymer materials. Designers should prioritize **recyclability, reusability, and material recovery** when selecting polymer architectures and product formulations.

Several strategies can support circular polymer design, including:

- Avoiding complex multi-material structures that hinder recycling
- Reducing the use of additives that interfere with recycling processes
- Designing polymers that are compatible with existing recycling infrastructure

- Incorporating degradable linkages or dynamic covalent bonds to enable chemical recycling or repair

Compatibility with sorting technologies, particularly **near-infrared (NIR) detection systems**, should also be considered during product development to ensure that materials can be effectively identified and separated in recycling facilities.

Where recycling is not feasible, biodegradable or compostable materials may provide alternative end-of-life pathways, provided that appropriate waste management infrastructure is available.

16.1.4 Minimize the use of hazardous additives

Polymer formulations often rely on additives to improve mechanical properties, processability, durability, or flame resistance. However, some additives historically used in polymer systems have been associated with toxicity or environmental persistence.

Best practices for **additive selection** include:

- Avoiding substances of very high concern (SVHC) whenever possible
- Substituting hazardous additives with safer alternatives
- Reducing additive loading through optimized polymer design
- Using reactive additives that chemically bond to the polymer matrix to prevent migration

In addition, the use of **bio-based fillers and reinforcement materials**, such as cellulose fibers, lignin, or biochar, can enhance material performance while reducing dependence on mineral resources.

When nanomaterials are used as additives, appropriate **nano-safety assessments** should be performed to evaluate potential health and environmental risks.

16.1.5 Optimize manufacturing processes for resource efficiency

Sustainable polymer innovation also requires improvements in manufacturing technologies. Polymer synthesis and processing operations often account for a significant portion of the environmental footprint associated with polymer products.

Best practices for **sustainable manufacturing** include:

- Implementing solvent-free or low-solvent polymerization techniques
- Reducing processing temperatures to minimize energy consumption
- Applying reactive extrusion and continuous processing technologies
- Using energy-efficient equipment and heat recovery systems
- Implementing closed-loop water management systems

Process intensification strategies and digital monitoring technologies can further improve efficiency and reduce environmental impacts during industrial production.

16.1.6 Use digital tools to accelerate sustainable material Innovation

Digital technologies are becoming increasingly important for accelerating polymer development under SSbD principles. Computational modeling, machine learning, and data-driven design platforms allow researchers to predict material properties and environmental impacts before synthesis takes place.

Digital tools can support:

- Molecular design and property prediction
- Screening of alternative polymer formulations
- Optimization of processing conditions
- Integration of sustainability metrics into decision-making frameworks

The use of digital tools also facilitates the integration of large datasets related to chemical hazards, environmental impacts, and regulatory requirements, enabling more informed design decisions.

16.1.7 Foster collaboration and knowledge sharing

The successful implementation of SSbD strategies requires **strong collaboration between industry, research institutions, regulatory agencies, and innovation ecosystems**. Polymer development involves complex interactions between chemistry, materials science, engineering, toxicology, and environmental science.

Collaborative platforms and shared databases can improve access to high-quality data and promote the exchange of knowledge across sectors. Initiatives that support open science, FAIR data principles, and multi-stakeholder partnerships are essential for accelerating sustainable materials innovation.

16.1.8 Invest in education and capacity building

Finally, the transition toward SSbD polymer innovation requires investment in **education and professional training**. Researchers and engineers must develop expertise not only in polymer science but also in sustainability assessment, toxicology, circular economy principles, and regulatory frameworks.

Universities, research centers, and training institutions should integrate SSbD concepts into academic curricula and professional development programs. This will ensure that future generations of scientists and engineers are equipped with the skills needed to design safer and more sustainable materials.



Figure 5. Schematic overview linking the challenges discussed in Chapter 14, the corresponding solutions proposed in Chapter 15, and the final operational recommendations presented above.

16.2 Final conclusions

The Safe and Sustainable by Design framework represents a fundamental shift in the way polymer materials are conceived, developed, and implemented in industrial applications. By integrating safety, environmental sustainability, functionality, and circularity into the earliest stages of material innovation, SSbD offers a comprehensive pathway toward more responsible and resilient polymer systems.

The analysis presented in this handbook demonstrates that sustainable polymer innovation cannot be achieved through isolated technological improvements. Instead, it requires an integrated approach that combines molecular design, green chemistry, sustainable manufacturing, circular product design, environmental assessment, and regulatory foresight.

At the same time, the implementation of SSbD principles presents a series of technical, economic, and regulatory challenges. These include the substitution of hazardous substances, the integration of life cycle assessment methodologies, the development of scalable sustainable manufacturing processes, and the alignment of innovation strategies with evolving regulatory frameworks.

Overcoming these challenges will require coordinated efforts across the entire materials innovation ecosystem. Research institutions, technology centers, industrial companies, policymakers, and educational organizations must work together to develop the tools, methodologies, and infrastructure necessary to support SSbD implementation.

Despite these challenges, the opportunities associated with SSbD polymer innovation are substantial. Advances in bio-based materials, digital design tools, advanced recycling technologies, and sustainable manufacturing processes are opening new pathways for the development of polymer materials that meet both performance requirements and environmental sustainability objectives.

In the long term, the widespread adoption of SSbD principles has the potential to transform the polymer industry, enabling the creation of materials that contribute to a circular economy, reduce environmental impacts, and support sustainable economic growth.

The transition toward safe and sustainable polymer systems will be a gradual process, requiring continuous innovation, collaboration, and learning. However, by applying the best practices and guidelines outlined in this handbook, organizations can play a key role in shaping the future of polymer materials and ensuring that polymer technologies continue to deliver value to society while protecting human health and the environment.

17 ANNEX

1 Challenges

The detailed answers given for the survey (**as explained in Chapter 14**) in relation to the SSbD strategy, segmented into general and specific challenges, are shown here.

1.1 General challenges

1.1.1 Innovation and technology

Main concern: To develop innovative technologies that enable the production of sustainable polymeric materials without compromising their functionality, while addressing a complex regulatory framework that is in constant change.

Difficulty: This requires significant investments in research and development to create new processes and materials that meet SSbD standards with a high uncertainty regarding potential changes in regulation.

Example of progress:

- The European Union's Horizon Europe Research and Innovation Framework Program has allocated funds for the development of sustainable technologies in the chemical sector. This implies R&D entities with the opportunity to develop research under publicly funded projects.
- Companies like DuPont have invested in advanced technologies to produce more sustainable and safer polymeric materials.

1.1.2 Substitution of Substances of Concern and relation to functionality

Main concern: To identify and replace hazardous chemicals in polymeric materials with safer and more sustainable alternatives without compromising their functionality.

Difficulty: Substitution requires a deep understanding of the chemical and physical properties of substances of concern and their potential alternatives. It is also necessary to evaluate the environmental and health impact of these alternatives throughout their life cycle.

Example of progress: Companies like BASF have developed sustainable alternatives for certain chemical additives, promoting innovation in this area³⁶.

1.1.3 Sustainable life cycle

Main concern: To ensure that polymeric materials are designed to minimize their environmental impact throughout their life cycle, from production to recycling or final disposal. The calculation of LCA analysis, CO₂ footprint or Water Footprint will become a reference to measure, compare and identify a graduation for sustainability measurement.

³⁶ <https://carboncredits.com/basfs-new-plastic-additives-reduces-co2-footprint-by-60/#:~:text=German%20chemical%20giant%20BASF%20announced%20the%20launch%20of,uses%20renewable%20feedstocks%20instead%20of%20fossil%20fuel-based%20feedstocks.>

However, nowadays this is far from the day-by-day operations of most companies so the implementation and concern will take time.

Difficulty: This requires the implementation of LCA, Carbon Footprint analysis (ISO 14067), and Water Footprint analysis (ISO 14046) methods that consider all environmental aspects, from the extraction of raw materials to the end of the product's useful life.

In terms of LCA assessments in the development of new materials, the challenge also lies in the **modelling of processes** in order to apply a model at the same time that material composition developments are taking place.

Examples of progress:

- Spanish Ministry of Environmental Transition has implemented a free access CO₂ footprint tool³⁷ and a recognized label for those companies applying the schema to push its use by companies across all sectors.
- Companies like IKEA have implemented programs³⁸ for recycling and reusing materials, reducing their environmental footprint.

1.1.4 Data access and collaboration

Main concern: To facilitate access to high-quality data and promote collaboration between actors to ensure the effective implementation of the SSbD strategy.

Difficulty: This requires the implementation of FAIR data principles (findable, accessible, interoperable, reusable) and collaboration between industry, academia, and regulatory agencies.

Example of progress:

- The European Commission is developing a common data platform on chemicals³⁹ to facilitate access to and exchange of information.
- Initiatives such as the European Innovation Alliance for the Circular Economy⁴⁰ promote collaboration between different sectors to advance in the sustainability path.

1.1.5 Education and training

Main concern: To ensure that professionals involved in the development of polymeric materials have the skills necessary to implement the SSbD strategy.

Difficulty: This requires the review and updating of educational curricula and training programs to include SSbD principles. Involve training centers (such as Universities,

³⁷ <https://www.miteco.gob.es/en/cambio-climatico/temas/registro-huella/huella-de-carbono/inscripcion.html>

³⁸ <https://www.ikea.com/global/en/our-business/sustainability/our-circular-agenda/?msockid=0219cc70434165a0201adec742e964d8>

³⁹ <https://echa.europa.eu/es/understanding-the-regulation-on-the-common-data-platform-and-monitoring-and-outlook-framework-for-chemicals>

⁴⁰ <https://www.cid-innovationalliance.eu/>

Colleges, private educational entities...) which are quite unflexible nor easy adaptable when introducing curricula changes.

Examples of progress:

- The European Commission has recommended that MS include education on sustainability in their national research and innovation programs.
- Universities and research centres have begun to offer specialized courses and programs in sustainability and green chemistry.
- EU calls, such as Erasmus+ program, are supporting some projects that aim to develop training programs for different levels of students and packaging companies' workers to be trained in sustainability and circular economy plastic packaging (e.g., the RESPA project⁴¹).

1.1.6 Regulation and Standards

Main concern: To align the standards for the development of polymeric materials with European regulations and recommendations on sustainability and safety, particularly PPWR (packaging and packaging waste regulation⁴²).

Difficulty: This requires active participation for reviewing and improving regulations, such as the European Commission's Recommendation on SSbD.

Examples of Progress:

- The European Commission has established a European assessment framework for safe and sustainable chemicals and materials by design⁴³.
- Companies and industry organizations actively participate in the review of regulations to ensure they are practical and effective.

1.1.7 Costs and economic viability

Main concern: To ensure that sustainable polymeric materials are economically viable and competitive in the market, particularly when upscaling from laboratory to industrial scale.

Difficulty: This requires conducting long-term cost-benefit analyses, considering the potential savings derived from reducing environmental impacts and improving public health. The raw material oligopolistic market trends can condition the economic competitiveness of some materials compared to their substitutes.

Examples of progress:

- The European Union has implemented policies to support the financing of the transition to a sustainable economy⁴⁴, such as the Sustainable Finance Strategy.

⁴¹ <https://respa-project.eu/>

⁴² <https://eur-lex.europa.eu/eli/reg/2025/40/oj/eng>

⁴³ https://environment.ec.europa.eu/strategy/chemicals-strategy_en

⁴⁴ https://finance.ec.europa.eu/publications/strategy-financing-transition-sustainable-economy_en

- Companies like LEGO have demonstrated that sustainability can be profitable in the long term by reducing operating costs and improving their brand image ⁴⁵.

In summary, overcoming these challenges requires an integrated approach that combines technological innovation, collaboration between sectors, education, and effective regulation.

1.2 Specific technical challenges

1.2.1 Processability

Nowadays, additives are used to improve the processability of recycled polymers, which often lose technical properties during recycling. Temperature effects during processing affect the properties of the recycled material. For this reason, additives are used to compensate/balance this loss of properties, resulting in improved processability. Most of these additives (**Chapter 7**) are **process aids**, anti-degradants (to inhibit degradation), fillers (for improved mechanical properties), curing agents (which help to form a three-dimension network structure), and coupling agents (to enhance the compatibility of components). They are needed to guarantee conversion processes in optimal conditions when dealing with recycled materials. The addition of additives in this case can be difficult to avoid.

The challenge here is related to balancing the need for adding such additives without compromising SSbD requirements.

1.2.2 Regulation and other environmental desirable goals

1.2.2.1 Microplastics: *The increasing regulatory attention towards microplastics represents a major technical and environmental challenge for the polymer industry. Commission Regulation (EU) 2023/2055 introduced restrictions on intentionally added synthetic polymer microparticles under REACH, requiring manufacturers to minimise releases throughout the product life cycle and to provide adequate information on use and disposal. In parallel, Regulation (EU) 2025/2365 reinforces sustainability and environmental performance requirements for materials and products placed on the European market, particularly regarding circularity, biodegradability and prevention of persistent pollution. In this context, polymer developers must consider not only the functionality and durability of materials, but also their potential to generate secondary microplastics through abrasion, fragmentation, weathering or end-of-life degradation.*

⁴⁵ <https://sustainabilitymag.com/articles/lego-h1-2024-results-growth>

1.2.2.2 DfD (Design for Deconstruction) vs. SSbD (Safe and Sustainable By Design): *Considering the plastic product value chain, different aspects need to be taken into account. Some are more relevant in the early stages, such as SSbD material selection, while others become more important at the end-of-use phase, such as reuse or deconstruction. Therefore, an integrated approach to ecodesign is required, one that incorporates these key aspects to provide a comprehensive product perspective.*

1.2.2.3 Recyclability: *Appropriate sorting capability is crucial to ensure the product's recyclability. Technologies such as near-infrared (NIR) reflectance spectroscopy—particularly line-scan systems, which often perform better than snapshot systems—are used to analyze materials and their behavior in terms of NIR recognition.*

1.2.3 Raw material from recycled polymers market evolution

Nowadays, the recycling polymers raw material market is facing a **crisis in terms of price evolution and regulation restrictions/obligations**. From a market pricing perspective, the downward trend in virgin raw material prices has reduced demand for recycled polymer feedstocks, thereby driving their prices down. The high correlation between virgin and recycled material prices in a market controlled by a few petrochemical companies becomes a major challenge as competitiveness depends highly on market price.

In addition to market dynamics, regulatory developments also influence the availability and price of recycled polymer feedstocks. Trade restrictions affecting the international movement of recyclable materials, such as import bans on recycled plastic flakes implemented by some countries, together with increasingly stringent end-of-waste requirements and quality criteria, reduce the volume of recycled materials available on the market. These factors directly affect supply, market stability and price evolution, creating additional uncertainty for companies relying on recycled polymers as raw materials.

One important trend in polymer recycling is the development of chemical recycling, including gasification (**Chapter 10.1**).

However, the significant investments required for these technologies may be hindered by low material prices, as this reduces their competitiveness in terms of investment versus returns and market value. Upscaling processes when developing new sustainable materials.

1.2.4 Upscaling processes when developing new sustainable materials

Scaling up from laboratory to industrial production is a critical step in bringing new sustainable materials to market. Beyond maintaining material performance during larger-scale processing, successful upscaling also depends on the availability and cost of key raw materials and intermediates. In the REPurpose project, BHET (bis(2-hydroxyethyl) terephthalate) was used during the upscaling of new materials. However, BHET is

currently expensive, not widely available on the market and difficult to produce in large quantities, which represents an important barrier to industrial-scale implementation.

1.2.5 Control of toxicity (ecotoxicity tests)

Both **compounding and polymerization** process phases need to be duly aligned with toxicity tests in order to guarantee that no dangerous/unsuitable substances can appear at any moment of the composition, use or production process (material and product point of view).

The lack of clear information and **continuously updated developments regarding substance regulations** - such as the recent identification of PFAS as toxic - along with the resulting changes to regulatory frameworks like REACH, makes it difficult to maintain a consistent process and to clearly identify which substances must be controlled or avoided at any given time.

The recent adoption of **Directive (EU) 2022/431**, which extends the scope of protection for workers to include reprotoxic substances, represents an additional and significant challenge in the development of new polymeric materials. For the first time, occupational exposure to reprotoxic agents is explicitly regulated under the framework previously limited to carcinogens and mutagens. This implies that material developers must systematically assess not only the toxicity and ecotoxicity of final products, but also the potential presence, formation, or emission of reprotoxic substances throughout polymerization, compounding, processing, and end-of-life stages. The requirement to anticipate and control reproductive toxicity risks increases the complexity of substance selection, impurity profiling, and process monitoring from the earliest R&D phases.

Moreover, the **transposition of Directive (EU) 2022/431 into national legislations** - such as, for instance, the Spanish Royal Decree 612/2024 amending Royal Decree 665/1997 - reinforces binding exposure limits, risk assessment obligations, and preventive measures at industrial level. This regulatory evolution obliges companies to integrate toxicological screening, exposure scenario analysis, and compliance verification into material design strategies under a SSbD approach. For innovative polymers, particularly those incorporating novel monomers, additives, or recycled feedstocks, ensuring full alignment with these new reprotoxic protection requirements may result in additional testing costs, longer time-to-market, and the need for continuous regulatory surveillance across MS.

1.3 REPurpose project-specific challenges

Along REPurpose project research, the project partners identified different challenges during the project that are summarized below.

1.3.1 Uncertainty in techno-economic and environmental assessments (TEA & LCA)

Methodological challenge: The innovative nature of the developed molecules and processes created significant difficulties in benchmarking industrial costs and modelling environmental impacts.

Context and impact:

- For TEA, the lack of industrial references for depolymerization enzymes and novel intermediates required extrapolation from related sectors, introducing uncertainty in industrial projections.
- For LCA, the choice of a prospective approach (future industrial-scale scenarios) required defining technological improvement pathways and external influencing factors under high uncertainty. Multiple plausible scenarios had to be defined and prioritized before analysis.

Addressing this challenge required careful coordination between technical developers and sustainability experts to ensure that modelling assumptions remained aligned with evolving process data, while clearly documenting uncertainty ranges to avoid misinterpretation of results.

1.3.2 Data availability, analytical complexity and experimental bottlenecks

Technical challenge: Several analytical and experimental constraints affected execution efficiency:

- Quantification challenges in enzymatic production (e.g., glycosylated forms complicating SDS-PAGE analysis).
- Need to develop alternative, activity-based assays to ensure reliable comparability.
- Limited availability of benchmark polymers for new-to-market materials.
- Small sample quantities in early stages, limiting end-user validation.

Impact: These factors delayed decision-making loops and reinforced the need for flexible experimental planning, internal contingency strategies, and early involvement of testing and end-of-life partners, even when prototype maturity was still limited.

1.3.3 Alignment of material development, prototyping and testing timelines

Technical and coordination challenge: One of the main challenges during project execution was the synchronization of material development cycles with product design, prototyping and testing activities.

Context and impact: The iterative nature of developing new polymeric materials required repeated adjustments in processing parameters, geometries, and tooling. In several cases, material batches did not consistently meet the required specifications (e.g., molecular weight variability during upscaling or delays in material sample delivery),

which slowed down prototyping and limited rapid design iteration. Additionally, delays in the supply of key raw materials (e.g., recycled PET streams) required the identification of alternative suppliers, impacting experimental timelines.

From a management perspective, this highlighted the intrinsic complexity of integrating experimental, low-TRL materials into product-oriented workflows, where downstream partners depend on predictable material performance and availability.

Beyond project execution, partners identified several structural barriers that may affect the transferability and industrial implementation of the proposed Best Practices.

1.3.4 Industrial scalability and process engineering constraints

Scalability challenge: While prototypes and pilot-scale materials demonstrated promising performance, scaling up to industrial volumes introduces several constraints:

- Ensuring consistent polymer molecular weight and material quality at large scale.
- Reliable sourcing of sufficient feedstock quantities.
- Removal of by-products (e.g., ethylene glycol) requires strong vacuum systems, which become increasingly complex and costly at larger batch sizes.
- Some depolymerization applications require high dilution and long residence times, leading to low industrial productivity and high utility costs.

Implication: Industrial plant engineering must be specifically adapted to REP materials. Early-stage process intensification and productivity optimization are essential to prevent techno-economic barriers at higher TRLs.

1.3.5 Economic competitiveness and market readiness

Market challenge: Bio-based or circular materials often face higher production costs compared to fossil-based alternatives. Their market uptake depends on:

- Willingness to pay a premium for sustainability.
- Government incentives or regulatory push mechanisms.
- Stable recycled raw material markets, currently affected by strong price correlations with virgin materials.
- Investment risks in emerging technologies such as chemical and/or enzymatic recycling when market prices are volatile.

Implication: Without policy support and stable regulatory signals, even technically successful materials may struggle to achieve large-scale market penetration.

1.3.6 Regulatory evolution and compliance uncertainty

Regulatory challenge: The evolving European regulatory framework (e.g., SSbD framework, REACH updates, restrictions on substances such as PFAS, reprotoxic substances, and microplastics) creates uncertainty for long-term material development strategies. In parallel, aligning SSbD requirements with other environmental objectives (e.g., DfD, recyclability, ecodesign) requires an integrated product-level approach.

Implication: Companies must anticipate regulatory evolution and integrate safety, toxicity and ecotoxicity testing throughout polymerization and compounding phases to avoid future reformulation needs.

1.3.7 Functional performance vs. sustainability expectations

Technical-market interface challenge: For certain applications, especially those involving biodegradability, there is a delicate balance between:

- Guaranteeing durability and performance during use.
- Providing clear and credible biodegradability timelines.
- Ensuring compatibility with existing waste management systems.
- Achieving proper sorting and recyclability (e.g., NIR detection).

Implication: Future implementation requires clear labelling, robust performance validation, and alignment with real waste infrastructure capabilities to ensure stakeholder and consumer acceptance.

1.3.8 Continuity beyond project lifetime

Sustainability of impact challenge: Ensuring the continuity of communication, dissemination and stakeholder engagement activities after project completion remains a challenge.

Implication: To guarantee long-term uptake of Best Practices, mechanisms such as sectoral alliances, standardization contributions, and integration into industrial guidelines must be pursued beyond the project duration.

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