European Commission

Strategic Research and Innovation Plan for safe and sustainable Chemicals and Materials

Research and Innovation

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European Commission
Directorate-General for Research and Innovation
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Strategic Research and Innovation Plan for safe and sustainable Chemicals and Materials

2022 Directorate-General for Research and Innovation

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Executive Summary

The Chemicals Strategy for Sustainability (CSS) announces a Strategic Research and Innovation Agenda in 2022. The current Strategic Research and Innovation Plan (SRIP) delivers on this announcement and highlights current research and innovation (R&I) areas crucial for accelerating the transition to chemicals and materials that are safe and sustainable.

This SRIP is a result of extensive consultations with different stakeholder groups and reflects the R&I needs flagged during these consultations. It provides a comprehensive outlook of R&I needs for chemicals and materials across their lifecycle, i.e., from production to (re)use, disposal and pollution remediation. Chapter 3 outlines the key enablers and cross-cutting aspects crucial for maximising the impact of future research. Chapter 4 lists the R&I challenges linked to the design phase and builds on the work done in developing the safe and sustainable by design framework for chemicals and materials. Chapter 5 focuses on safe and sustainable production processes. The use stage of chemicals and materials requires R&I to enable a reliable assessment of functionality, performance, safety and sustainability, including exposure monitoring and modelling (Chapter 6) as well as hazard (Chapter 7) and risk assessment (Chapter 8). R&I needs related to the end of life of chemicals and materials emerging from the need to decontaminate and remediate pollution are addressed in Chapter 9. Chapter 10 sets out a monitoring scheme for the SRIP implementation.

The aim of the SRIP is to guide R&I funders in their decisions on investments across EU, national and private funding programmes. It is an opportunity for a more transparent communication among all relevant actors on joint R&I priorities proposed by the wider community: from academia to SMEs, large-scale industry, regulators and policymakers.

The Commission will refer to this SRIP in the Horizon Europe work programme as an overarching strategy. In addition, the Commission invites research and innovation funders across EU, national and private funding programmes as well as researchers and innovators to support this strategy and to contribute to its implementation.

1

Introduction

With the European Green Deal[1], the European Commission positions Europe to become the first climate neutral continent by 2050. The Green Deal defines four interlinked policy goals which will drive the transition to a sustainable economy and society: climate neutrality, biodiversity protection, circular economy and a zero-pollution ambition for a toxic-free environment. To achieve these, several strategies and action plans were adopted[2], amongst which is the Chemicals Strategy for Sustainability (CSS)[3]. The CSS aims to tackle the challenge of producing and using chemicals to address societal needs whilst respecting the planetary boundaries[4] and avoiding harm to humans and the environment. Addressing this challenge becomes even more urgent in the context of the increasing complexity of manufacturing and supply chains for some chemicals and materials[5], and the resulting need for the EU to secure access to those substances that are essential for our life and health and for achieving a climate-neutral and circular economy[6]. Thus, developing a strategic approach to research and innovation (R&I) for safe and sustainable chemicals and materials is not only a societal and planetary urgency but is also an economic opportunity for the EU's chemical industry to gain competitive advantage and to win consumers' confidence by investing in more sustainable solutions.

The CSS announces a Strategic Research and Innovation Agenda in 2022. The present Strategic Research and Innovation Plan (SRIP) delivers on this announcement and highlights the R&I areas crucial for making chemicals and materials safe and sustainable. This encompasses improving the overall sustainability of feedstock sourcing and production processes and technologies to allow the chemical industry's transition to climate neutrality and the

1 The European Green Deal
2 European industrial strategy, Zero Pollution Action Plan, EU Biodiversity strategy for 2030, Farm to Fork Strategy, EU Soil Strategy, Circular Economy Action Plan, the Hydrogen Strategy, Materials 2030 Manifesto
3 Chemicals Strategy for Sustainability
4 Is Europe living within the limits of our planet? An assessment of Europe's environmental footprints in relation to planetary boundaries
5 EU strategic dependencies and capacities: second stage of in-depth reviews
6 Commission Staff Working Document: Strategic dependencies and capacities

zero-pollution ambition. This document aims to provide a comprehensive outlook of the key R&I needs for chemicals and materials across their lifecycle, i.e., from production to (re)use, disposal and pollution remediation (Fig.1). This SRIP is a result of extensive consultations with different stakeholder groups and reflects the R&I needs flagged during these consultations (see Chapter 2).

This document does not distinguish between base and specialty chemicals and the terms 'chemicals' and 'materials' are used generically, unless otherwise specified, to cover all substances, including special categories such as metals, polymers, nanomaterials and other categories.

As the production of chemicals and materials is energy and resource-intensive some of the identified research and innovation gaps are not unique for the chemical industry but rather cross-cutting for energy-intensive sectors and processes. Therefore, additional funding to improve the overall sustainability of industrial production has been already mobilised in relevant Horizon Europe partnerships[7]. Moreover, other initiatives complement the SRIP by tackling challenges related to the impact of pollution on environmental and human health, e.g., Horizon Europe Missions[8], or by presenting the state of play of relevant key technologies and available support instruments, e.g., the ERA industrial technology roadmaps[9] and the Transition Pathway for the EU Chemical Industry[10] for the chemical sector.

The present SRIP will support another R&I action announced in the CSS – the safe and sustainable by design framework[11]. This framework sets out an approach to assess the safety and sustainability of a chemical or material across its lifecycle. Tackling R&I needs identified in the SRIP will support the safe and sustainable by design framework through e.g., innovative methods and models, better data availability for the assessment and innovation for the transition to safer and more sustainable production processes and end-of-life options.

Given that chemicals and materials affect almost all aspects of development, the SRIP will support several of the UN's Sustainable Development Goals (SDGs). In particular, SRIP supports the sound management of chemicals and waste – a specific target of SDG 12 on Sustainable Consumption and Production, and which is also referred to by SDG 3 on Good Health and Well-being and SDG 6 on Clean Water and Sanitation. More broadly, safe and sustainable chemicals and materials are crucial for achieving goals in the area of food security (SDG 2), health (SDG 3) and sustainable cities (SDG 11). Enabling safe and sustainable production processes and technologies may help to achieve SDG 9 on Industry, Innovation and Infrastructure.

By identifying the important R&I areas for making chemicals and materials safe and sustainable the SRIP will help to guide research and innovation funders in their decisions on investments.

7 European Partnerships
8 EU Missions in Horizon Europe
9 ERA Industrial Technologies Roadmap
10 European Industrial Strategy
11 Safe and sustainable by design framework

To monitor the SRIP impact the Commission will produce an overview of how much Horizon Europe funding is dedicated to R&I activities related to chemicals and materials in overall, as well as with a breakdown of funds according to the technical chapters of the SRIP. This overview will give guidance regarding existing investment gaps and thus help to prioritise actions for closing them to achieve the CSS's policy goals and improve the overall European science-policy interface. This is accompanied by an open invitation to other EU or national programmes to make use of the methodology to be proposed (Chapter 10) and to contribute to the overall reporting.

The SRIP is organised in eight scientific chapters. Chapter 3 outlines the **key enablers and cross-cutting aspects** crucial for maximising the impact of future research. Chapter 4 lists the R&I challenges linked to **the design** phase and builds on the work done in developing the safe and sustainable by design framework for chemicals and materials. Chapter 5 focuses on safe and sustainable **production processes**, including R&I needs to increase safety, energy efficiency and resource efficiency/circularity. The **use stage** of chemicals and materials requires R&I to enable a reliable and robust assessment of functionality/performance, safety and sustainability, including exposure monitoring and modelling (Chapter 6) as well as hazard (Chapter 7) and risk assessment (Chapter 8). R&I needs related to the **end of life** of chemicals and materials emerging from the need to decontaminate and remediate pollution are addressed in Chapter 9. Chapter 10 sets out a monitoring framework with R&I indicator to monitor the SRIP's implementation.

Figure 1: The life-cycle approach of the Strategic Research and Innovation Plan (SRIP)

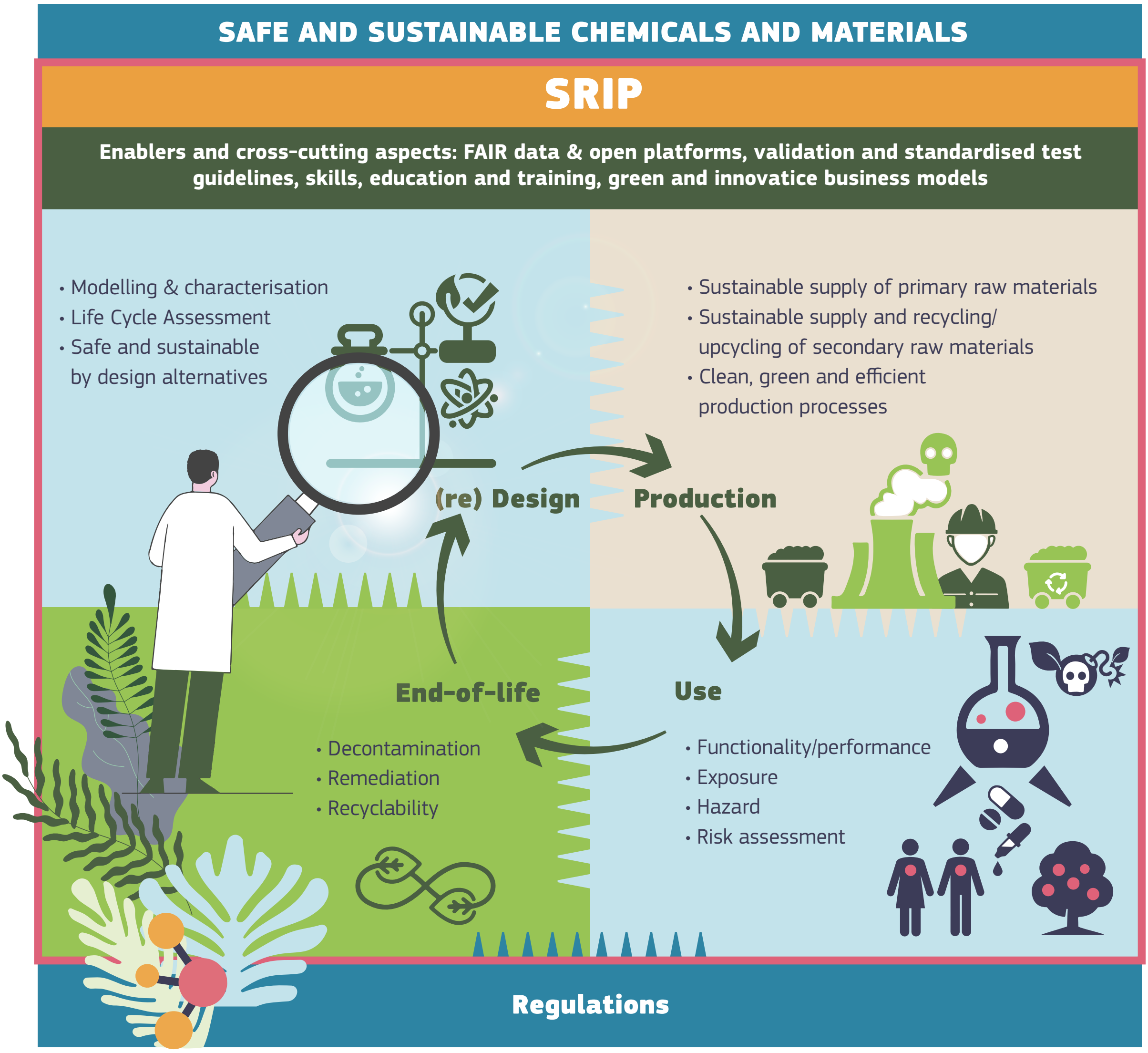


***Figure 1**: The life-cycle approach of the Strategic Research and Innovation Plan (SRIP). The Plan focuses on enabling and crosscutting aspects and R&I needs in line with life cycle stages of chemicals and materials. As chemicals and materials are used in many different sectors and consumer goods the identified R&I areas can also contribute to increasing the overall sustainability of these value chains and products.*

2 Stakeholder consultations

This R&I plan is a result of co-creation between the European Commission's Directorates-General, relevant EU Agencies and a wide network of stakeholders from many different areas. Ensuring an appropriate consultation mechanism by engaging a broad range of stakeholders throughout the development of the Strategic Research and Innovation Plan (SRIP) allowed for channelling their scientific and technical advice to this report, which is available to policymakers.

The first round of stakeholders' consultation, from December 2021 to January 2022, involved the R&I community (partnerships, existing technology platforms, associations and EU Agencies and their stakeholder groups) and focused on the vision and outline of the SRIP and the main research challenges under these. Consolidated input was provided by selected groups that represent academia, industry including SMEs, NGOs and Member States (via the European Chemical Agency (ECHA), European Food Safety Authority (EFSA) experts and Member States networks).

A second open consultation occurred in June 2022. During this consultation stakeholders were asked to identify any major missing R&I needs, correct wrong attributions of R&I needs between the different chapters and flag any specific factual or terminology errors. All collected comments were analysed and served as input for refining and finalising the SRIP.

In addition, at the meeting in May 2022 of the High-Level Roundtable on the Implementation of the Chemicals Strategy for Sustainability the topical focus was R&I for the transition to safe and sustainable chemicals and materials. This resulted in the Joint Report on Research & Innovation and Safe and Sustainable by Design[12]. Recommendations from this report have been duly considered.

12 Joint Report on Research & Innovation and Safe and Sustainable by Design

3

Enablers and cross-cutting aspects

There are several cross-cutting aspects to the different R&I needs covered in this document. Ensuring access to quality data and validated innovative tools will be fundamental to speeding up innovation. Coherent standards at the European level will facilitate the deployment and uptake of these new tools. Boosting education and skills will be critical for training a new generation of researchers and enhancing sustainability management in industry, including SMEs. Finally research into new business models will be key to support the transition of the industry to safe and sustainable chemicals and materials.

3.1. FAIR data and open platforms

There is a lack of findable, accessible, interoperable and reusable (FAIR) data on the use and occurrence of many chemicals, on chemical flows along value chains and on exposure of humans and the environment. Access to information on chemicals, their toxicological properties and their presence in the environment has improved considerably, e.g., through REACH[13], the Information Platform for Chemical Monitoring (IPCHEM)[14]; the Life Cycle Data Network[15], the European Food Safety Authority's (EFSA) new open access platform[16] and the efforts of the European Environment Agency (EEA). However, scientists, risk assessors and risk managers still find themselves confronted with gaps in knowledge and the lack of interoperable, high-quality data across the life cycle,

13 REACH
14 Information Platform for Chemical Monitoring
15 European Platform on Life Cycle Assessment
16 EFSA's new open access platform

which hampers the assessment of the safety and sustainability of chemicals and materials.

Apart from data ownership and confidentiality, a lack of data harmonisation remains a significant barrier for data sharing for both research and regulation. The European Open Science Data Cloud[17] provides guidance and support for data sharing. The Chemicals Strategy for Sustainability (CSS) announces the development of an open chemicals data platform in support of the 'one substance one assessment' approach[3].

Research and innovation is needed in the following areas:

- **Open platforms**: ensure seamless access and combination of data and tools (e.g., methods and models) from different databases enabling exchanges between different stakeholders respecting the General Data Protection Rules (GDPR), protection of Intellectual Property Rights (IPR), Confidential Business Information (CBI) and access rights in line with European data governance act[18]; stimulate open information exchange along value-chain actors on safety and sustainably aspects to facilitate risk assessment and enable the creation of new business opportunities across the innovation ecosystem.

- **Big data tools**: enable the use of large volumes of both structured and unstructured data to support hazard and risk assessment, early warning signals as well as safe and sustainable by design (SSbD) approaches; facilitate the efficient extraction of data from legacy documents, assessment and curation of data quality and interpolation of gaps; enable algorithmic assembly of datasets and models across multiple domains to provide comprehensive information on the use, exposure and effects on humans and the environment during the entire life cycle; develop artificial intelligence-based methods for the assembly of life-cycle inventories and for forecasting scenarios over multiple time and spatial scales; develop data visualisation tools to support decision-making and improve communication.

- **Data interoperability and management**: improve harmonisation and interoperability of databases and allow data re-usability for different tools for SSbD, exposure, hazard, risk and life cycle assessments; develop harmonised, domain specific ontologies for data documentation; develop harmonised frameworks and user-friendly tools for reporting and sharing data and metadata related to safety and sustainability assessments; implement data quality approaches and uncertainty analysis.

17 European Open Science Data Cloud
18 European data governance act

3.2. Validation and standardised test guidelines

More efforts are needed to map regulatory needs and provide access to a wider range of relevant tools for regulators, ensure uptake of innovative research results and facilitate the use of animal-free test methods. For test methods and tools to be usable for regulatory purpose, inter-laboratory validation and international standardisation are needed. While the OECD's process to develop Test Guidelines (TGs) and Guidance Documents (GDs) on chemical safety testing is time and resource consuming, with Good Laboratory Practise (GLP) they form the basis of the Mutual Acceptance of Data which is essential for all regulatory assessments of chemical safety within the EU. Therefore, the OECD's work is an indispensable contribution to a strong and enforceable EU regulation. The Malta Initiative[19] is adapting existing and developing new OECD TGs and/or GDs for regulatory requirements for nanomaterials. The public-private PEPPER platform[20] supports the pre-validation of testing methods on endocrine disrupting chemicals. However, there are currently a large variety of New Approach Methodologies (NAMs) that need validation. Actions for development and standardisation and TGs should engage different actors (e.g., national agencies, research institutes and industry), to coordinate efforts and build synergies. Another area where standardised tests are also needed is for the assessment of a material's durability (e.g., wear during the use phase). Validated and standardised tools and methods should be easily accessible to all users, especially for the SMEs.

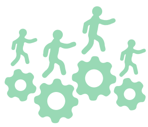
Research and innovation is needed in the following areas:

- **Validation of methods**: extend the number of validated methods, including NAMs addressing both health and environmental safety, thus also leading to more OECD TGs, in particular for complex materials; establish guidance on data integration of the different NAMs; enhance collaboration projects with regulators/authorities and researchers for the regulatory use and acceptance of NAMs and other new methods; develop a set of criteria for the regulatory acceptance of NAMs; compare the uncertainties arising from the different NAMs with the uncertainties arising from in vivo studies; support the lab-to-lab transferability of methods for validation and incentivise companies to share test methods and data developed in-house; improve quality control process in laboratories, in line with EU GLPs[21].

- **Reference materials**: develop and make accessible reference materials (including for complex materials), as well as reference data (e.g., mass spectra) harmonised protocols and quality requirement for non-targeted screening (NTS).

19 The Malta Initiative
20 PEPPER platform
21 EU Good Laboratory Practices

- **Durability tests**: standardise accelerated testing protocols and devices to assess, among others, the friction, wear, corrosion, or fatigue behaviour of materials.



3.3. Skills, education and training

To successfully achieve the green and digital transition it is vital to foster the skills and competences needed. A good example is the European Institute of Innovation and Technology (EIT[22] and the EU-funded Knowledge and Innovation Communities, e.g., the Climate-KIC[23]. Transition Pathway for the EU Chemical Industry[10] (under development) has identified a number of actions for skills, education and training, which go hand in hand with the needs identified here. The European Research Area also promotes the upskilling and reskilling of talent, especially in academia[24] and foresees several actions to develop sustainability skills. Needs identified here are specifically linked to the present R&I context.

Research and innovation is needed in the following areas:

- **Integrated approach in academic training**: establish curricula encompassing education in chemistry, physics, materials research and engineering with environmental, social and economic dimensions, as well digital skills and behavioural science; enable new generations of the workforce to act and make decisions based on a deep understanding of the complex relationships between scientific and technological activities, society and the environment; establish education tools/programmes on SSbD to enhance safe and sustainable chemicals and materials as well as NAMs for the transition to animal-free testing.

- **Stronger academia-industry collaboration**: bring academia and industry (including SMEs) together to exchange knowledge and better meet the R&I needs of companies. Develop skills and competences to address demands from the private sector and from risk assessment institutions and build a community with a strong understanding of the nexus between chemistry, materials science, product design, and sustainability.

- **Societal education**: develop educational materials including training programmes for open risk communication, debate and dialogue, and case studies training programmes for different stakeholders, including consumers, environmental justice groups, NGOs or entrepreneurs.

22 European Institute of Innovation and Technology
23 EIT Climate-KIC
24 European Skills Agenda

3.4 Green and innovative business models

Beyond the role of technology, innovation in business models is another important driver for the green transition of upstream and downstream industry and businesses. The transition to a circular economy and the foreseeable convergence with digital technologies in many fields may lead to disruptive changes along the value chains. By putting the performance/service the chemicals deliver at the centre of the business, new business models will turn the economic goal from selling as much as possible into providing the service with optimised resource efficiency. Thus, these models will be turning 'efficient use of chemicals' into an economically driven goal throughout the whole supply chain. Innovative business models should optimise the use of available expertise, ensure resource efficiency and the better management of hazardous chemicals during the entire life cycle and encourage place-based, local innovation and the involvement of SMEs. The industrial and industrial/urban symbiosis is a concept that allows businesses to take competitive advantage of the circular use of materials, energy, water and/or by-products in traditionally separate industries and urban ecosystems. The key for this symbiosis is the collaboration and the synergetic possibilities offered by geographic proximity.

Research and innovation is needed in the following areas:

- **Leasing or service**: establish leasing or service models for the chemical industry to change from volumetric supply of chemicals and materials, entailing cooperation along the complete value chain; establish clear and performance-related functional units (unit of payment) based on best practices to facilitate these new business models; establish industry specific roadmaps and milestones for 'how to move to chemical as a service' in the most efficient and inclusive manner.

- **Best practices and knowledge base**: develop best practices guidance for integrated waste management in line with the legal requirements leading to a circular economy. Support knowledge development in change management, develop instructions for how to design profit sharing and liability issues.

- **Tracking systems**: elaborate collaboration models with the involvement of all the actors in the value chain and across markets (from the chemical industry to formulators, manufacturing industry and recyclers) with the involvement of the IT industry and standardisation actors to improve tracking, quality control, monitoring and documentation and maintenance of chemical elements across values chains and thereby create new markets.

- **Circular approaches**: create innovative value chains that leverage industrial and industrial-urban symbiosis with the objective to maximise the circularity of resources (chemicals, materials, energy and water) in a regional/local ecosystem (i.e., Hubs4Circularity[25]); co-design specific implementation strategies, ensuring the participation of all stakeholders (industry, SMEs, research and technology organisations, local authorities, educational institutions and civil society).

25 Hubs4Circularity

4

Safe and sustainable by design

To reduce the negative impact of chemicals and materials on ecosystems and people, holistic approaches considering long term safety and sustainability aspects along the lifecycle are needed. The safe and sustainable by design (SSbD) framework aims to evaluate safety and sustainability through the whole life cycle during the development of chemicals and materials. Although significant progress has been made[26,27,28], further methodological advancements are needed to support the SSbD framework[11] and to allow for a coherent assessment, including the handling of trade-offs and uncertainties and exploring the full potential of the framework to drive innovation.

Toolboxes are needed to drive the uptake of SSbD and provide access to a combination of methods and models. Tools need to be accompanied by access to interoperable data from across the value chain, and by information about the reliability of data and tools. Toolboxes should be accessible to all stakeholders, in particular to SMEs, to help foster innovation.

4.1. Modelling and characterisation

Models and advanced characterisation play an important role in the design of chemicals and materials. To support the assessment of performance and functionality molecular modelling can be applied to quantitatively describe and predict physical and chemical characteristics of systems. Advancements in digital technologies such as high-performance and quantum computing will boost the analytical capacity of the models. This will render the R&I cycle for SSbD materials and chemicals more efficient and effective. All models need to include methods for the quantification of uncertainties and high quality input data must be ensured.

26 Mapping study for the development of sustainable-by-design criteria
27 Safe and sustainable by design chemicals and materials. Review of safety and sustainability dimensions, aspects, methods, indicators, and tools
28 Safe and sustainable by design chemicals and materials. Framework for the definition of criteria and evaluation procedure for chemicals and materials

Research and innovation is needed in the following areas:

- **Characterisation**: advance analytical techniques for the characterisation of chemicals and materials to guarantee high quality data; develop models for multi-modal, multi-scale and multi-dimensional phases (i.e., representations of the possible states of the system) for the characterisation of chemicals and materials; develop models for assessing similarity in safety and sustainability performance and properties of chemicals and materials.

- **Optimisation**: develop more robust, interoperable and adaptive models for multi-objective optimisation of different requirements for a chemical or material e.g., performance, functionality, safety and sustainability; develop models of functionality and required amount for a chemical in a given use.

- **Prediction**: establish models for specific matrices for the assessment of the impact of chemicals and materials (e.g., fate and transformation) and connect these to the in-silico simulation tools to assess the influence of the chemicals and materials on people and the environment; develop simulation tools generating future scenarios predicting the functionality, performance, safety and sustainability of new chemicals and materials and the processes needed to produce and recover them.

- **Design**: develop models that provide alternatives during the design phase and create a database of suitable safer alternatives, considering future regulatory requirements; develop models taking into account findings from the recycling and disposal of existing chemicals and materials to redesign chemicals and materials from secondary raw materials to achieve the same or enhanced functionalities.

- **Processes**: elaboration of modelling services for the precise analysis of the process to allow an efficient scale up of the processes from lab to production scale.

- **Data gaps**: improved methods to address missing data, e.g., extrapolating and upscaling, with advanced technologies like artificial intelligence or deep learning.

4.2. Life-cycle assessment

The hazard properties of a chemical, material or product may have consequences along the whole life cycle. Due to environmental and/or process conditions, a chemical or material may evolve and present different hazardous properties. By adding aspects of the life cycle in the simulation of the design phase (e.g., processing, use, recycling), a holistic assessment of the impact of a chemical or material can be performed. Currently, the knowledge on the overarching life-cycle hazard and exposure assessment for both chemical and materials is scarce. Increasing interest in sustainability has led to the development of many sustainability assessment tools (e.g., Life Cycle Analysis (LCA), Life Cycle Costing and Cost–Benefit Analysis). However, the methodological disparity of these tools can lead to conflicting assessment results and generate confusion for many policy and business decisions. Thus, alignment across social, economic and environmental domains still needs further improvement. Multidisciplinary approaches should be built on a methodological framework that considers the entire lifecycle of chemicals and materials throughout their value chains, addressing circularity and understanding the mechanisms and actors at the origin of the risks as well as economic, environmental and societal implications.

To address these issues, the Commission created the European Platform on Life Cycle Assessment[29] which serves as the EU's knowledge base that responds to business and policy needs towards sustainable production and consumption.

Research and innovation is needed in the following areas:

- **Analytical frameworks**: develop analytical frameworks integrating the principal impacts (environmental, social and economic) that are typically considered in LCA as well as chemical safety indicators when possible; ensure better integration of multiparametric toxicity/risk assessment with LCA methodologies; better address the feedstock transition and especially the complexity of different types of renewable carbon feedstock (e.g., CO_2, plastics waste, biomass).
- **Transformation assessment**: develop test methods and analytical tools to assess transformation of substances via various (a)biotic processes including mass balance; improve environmental representativeness across all life cycle stages, with special attention to use and end of life as well as to difficult to test substances (e.g., endocrine disrupting substances, persistent, bioaccumulative and toxic (PBT) substances and persistent, mobile and toxic (PMT) substances or advanced materials such as nanomaterials.
- **Models and data for production, use and recycling**: generate data and develop models to represent chemical or material production and life cycle stages prior to the production (e.g., the extraction of raw materials) as well as chemical use and recycling across the whole value chain.
- **Prospective assessment**: develop methods for the estimation of environmental impacts of new technologies and suitable for the various stages of development of chemicals and materials.
- **Integrated risk and life cycle assessment**: advance methods to integrate risk and life cycle assessment; develop guidelines to assess trade-off for decision makers.
- **Impact indicators**: develop indicators to assess the impacts and drivers of chemical pollution through the life cycle of a substance building on available experience in the areas of air, water, marine, soil and biodiversity; estimate planetary boundaries on key impact indicators and support moving towards absolute sustainability.

29 European Platform on Life cycle assessment (EPLCA)

- **Tools for socio-economic assessment**: develop tools to assess, quantify and, where possible, monetise benefits and costs, including externalities to human and environmental health, as well as other socio-economic aspects and identify most cost-effective solutions; develop cost categories for specific groups of substances, e.g., social cost of persistent chemicals (analogous to the social cost of carbon used in climate economics); develop methods for the quantification of emerging impacts and for the estimation of non-quantifiable impacts; achieve wider stakeholder agreement on these innovative tools.

4.3. Development of safe and sustainable by design alternatives

To encourage uptake and emphasise the advantages of applying the SSbD framework proposed by the European Commission, good case studies of substitution of the most harmful substances are needed. Substitution should aim at developing safe and sustainable alternatives that provide the same or enhanced functionality with lower toxicity and hazard (or even non-toxic, non-hazardous) profiles and with improved sustainability performance. SSbD chemicals and materials have the potential to contribute to new applications of advanced materials within the innovation markets identified in the Materials 2030 Manifesto[30]. For all the research areas production and scale up challenges should be addressed as well as efficient dissemination of information on safe and sustainable alternatives.

The focus of this section is the application of the SSbD concept to find alternatives to the most harmful substances as a priority for action. However, this approach does not limit the overall objective to implement the SSbD framework in the development process of all chemicals and materials as well as finding non-chemical alternatives.

Research and innovation is needed in the following areas:

- **SSbD flame retardants**: develop new flame retardants without hazard profiles that would lead to classification as Substances of Very High Concern (SVHCs), e.g., medium-chain chlorinated paraffins or halogenated flame retardants, or materials that in other ways prevent or retard flames, e.g., by blocking access to fire, oxygen or channel heat away; target several application areas such as construction, transport or consumer products.

30 Materials 2030 Manifesto

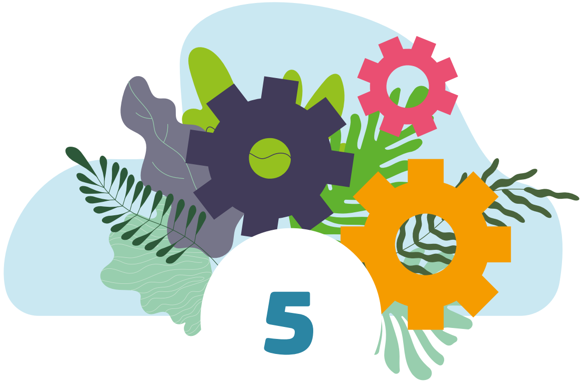
- **SSbD materials with plastic like properties**: develop new materials, including biodegradable alternatives, maintaining similar or enhanced functional properties (e.g., flexibility, durability and/or toughness) that are sufficient for the intended service and expected use (time, chemical or physical stress) as existing plastics. This can include alternatives to additives that are substances of concern, such as phthalates and bisphenols.

- **SSbD surfactants**: develop new surfactants addressing safety aspects along the entire life cycle and explore alternative feedstocks for increased sustainability.

- **SSbD solvents**: develop solvent formulations without hazardous substances and toxicity aspects linked to their volatility and risks of pollution along their entire life cycle.

- **SSbD corrosion and fouling-resistant materials**: develop new treatments or new materials inherently resistant to corrosion and fouling for the intended time of use, as alternatives to current surface treatment applications.

- **SSbD plant protection and/or biocidal products**: develop new plant protection and biocidal products with improved efficiency, biocompatibility and biodegradability to overcome the problems of traditional agrochemicals.



5 Safe and sustainable production processes and technologies

Chemicals and materials production is an energy and resource-intensive process that has important impacts on pollution. The green and digital transition, as aimed for in the European Green Deal, still requires significant advances to achieve climate neutrality goals and the zero pollution ambition for a non-toxic environment[31]. Significant gaps remain on how to overcome technical and scientific challenges for clean and smart production processes progressing towards carbon neutrality and maximising resource efficiency, and to ensure access to sustainable primary and secondary raw materials and increase circularity. The revision of the Urban Wastewater Treatment Directive[32] and the Industrial Emissions Directive[33] will modernise these regulatory frameworks and foster innovation. Clean and smart production processes are also relevant to increase the protection of workers exposed to hazardous substances[34], which is the focus of several EU regulations[35,36].

The sharing of best practices and developing synergies amongst sectors is also important. The new Innovation Centre for Industrial Transformation & Emissions (INCITE) will help industry identify pollution control solutions. As stated in the introduction, many of the challenges faced by the chemical industry are not unique to this industry and several activities are already ongoing to decarbonise industry and support the green transition of energy intensive industries. To achieve sustainable chemicals and materials the chemical industry will be

31 Zero Pollution Action Plan
32 Urban Wastewater Treatment Directive
33 Industrial Emissions Directive
34 EU strategic framework on health and safety at work 2021-2027
35 Directive on the protection of the health and safety of workers from the risks related to chemical agents at work
36 Directive on the protection of workers from the risks related to exposure to carcinogens or mutagens at work

interlinked with advances in other sectors and therefore the following R&I needs identified by stakeholders might go beyond the chemical industry as such.

5.1. Sustainable supply of primary raw materials

A sustainable supply of primary raw materials is necessary to prevent their shortage for future generations. The demand for primary raw materials is shifting due to new consumer patterns and new technologies that allow for the substitution of non-renewable and energy intensive materials and catalysts. The sustainability dimension of a primary raw material starts from their sourcing. The sustainable sourcing and use of primary raw materials require that safe materials or materials that can be safely and sustainably processed are generated with minimal or zero impact on other resources. Sustainable sourcing considerations should include low/zero Indirect Land Use Change (ILUC) impacts, practices to assess and prevent biodiversity loss and ecosystem degradation as well as social and ethical considerations and trade-offs (e.g., between various ecosystem services, competing use of biomass)[37].

The European Alliance for raw materials addresses these challenges for rare earths and magnet value chains. However, the chemical (and processing) industry is faced with a wider need for primary raw materials, in particular the reduction of dependency on fossil feedstock and overall feedstock diversification. Moreover, the energy used for the acquisition and processing of the primary raw material must be produced sustainably, the process energy efficiency must be maximised and the emission of greenhouse gasses as well as pollution must be minimised or avoided.

Research and innovation is needed in the following areas:

- **Sustainable access to raw materials**: enhance efficiency, occupational safety and sustainability, beyond best available techniques, of the different steps involved in extraction and processing of minerals and metals such as flotation, grinding and separation; develop refining or separation processes using fully recyclable, green solvents.
- **Sustainable access to biomass**: develop new technologies for safe, cost-effective, sustainable and feasible sourcing, logistics and valorisation of biomass from different territories (land, freshwater, sea).
- **Renewable syngas production**: develop new technologies for syngas production from renewable resources.
- **Renewable hydrogen production**: improve all renewable technologies that can produce clean/low carbon hydrogen (e.g., water electrolysis using renewable energy, methane pyrolysis); develop technologies to increase biogas production; develop

37 A sustainable Bioeconomy for Europe. Strengthening the connection between economy, society and the environment

innovative approaches in the supply chain to ensure safe and competitive hydrogen supply.

- **Alternatives for rare raw materials**: develop alternatives for rare raw materials applications at a component level, including energy harvesting, electromobility and energy storage.

5.2. Sustainable supply and recycling/upcycling of secondary raw materials

Currently a very limited amount of the material resources used by the European process industry is composed of recycled and recovered materials and these are mostly downcycled to less valuable products. To move towards a more circular and sustainable industry that uses its resources strategically, which follows the waste hierarchy with no landfilling, the recycling and preferably upcycling of large amounts of secondary resources is needed. The chemical industry holds a key role in this aspect as many of its products are the raw materials for other sectors. In a clean circular economy, it is essential to boost the uptake of secondary raw materials and ensure that both primary and secondary materials and products are safe to use in their intended applications. The circular economy action plan 2.0[38] has shown that this requires a combination of actions upstream, to ensure that products are safe and sustainable by design, and downstream, to increase safety and trust in recycled materials and products. To reach this aim there is a need to foster findable, accessible, interoperable and reusable (FAIR) data and digital assets principles. One contribution to the way forward is the application of a Digital Product Passport (DPP)[39] between recycling companies and the process industry to improve the economies of scale in upcycling of material streams.

5.2.1. Recuperation and recycling/upcycling of waste

Research and innovation is needed in the following areas:

- **Measurement of substances in waste streams**: develop analytical tools to identify and quantify substances in complex waste mixtures (e.g., plastic waste, electronic equipment waste, construction waste, windmills, batteries) including rapid sensing technologies.

- **Sorting and separating**: develop efficient solutions for sorting of waste and for separation of hazardous substances at all levels in the supply chain from the very beginning of the production processes until end of life, including the foreseen dismantling and recovery processes; develop extractive and processing technologies for improved separation of by-products.

38 Circular economy action plan 2.0
39 On making sustainable products the norm

- **Wastewater treatment**: develop advanced industrial and urban wastewater treatment technologies beyond Best Available Techniques (BATs) for energy, solute and nutrient recovery as well as for the removal of chemical contaminants.

- **Upcycling and recycling**: develop efficient recycling strategies that address the specific needs of solid waste e.g., plastic waste, biomaterials, nanomaterials, such as physical, chemical and biological recycling for pure and mixed plastic waste in closed loops and avoidance of downcycling; target recycling of critical raw materials (such as lithium, rare earth metals and other rare inorganics); develop technologies for the efficient use of by-products from wood refining, and for recovery of primary raw materials from farm production and associated waste streams; increase knowledge on the performance, durability and energy efficiency of secondary raw materials to assess viability of recycled materials.

- **Residue treatment**: develop technologies for residue treatment (e.g., chemical recycling, thermal processing), establish controlled sink of hazardous components from old material recycling, enhance landfill mining.

- **Valorisation of soluble compounds**: develop conversion technologies that transform solubilised compounds to valuable chemicals (e.g., in situ generation of chemicals from liquid waste streams by advanced membrane technologies).

- **Valorisation of secondary, residual and waste biomass**: develop technologies to converse effectively and sustainably secondary, residual and waste biomass to fuels and value-added chemicals.

- **Monitoring and mapping**: develop advanced mapping, tracking and tracing of materials across the supply chain, and improve data completeness, accuracy and interoperability between the industrial processes and the recycling companies, promoting the application of the DPP; develop efficient information mapping and sharing system for secondary resources to promote secondary raw materials markets.

5.2.2. Valorising emissions

Research and innovation is needed in the following areas:

- **Carbon capture, utilisation and storge**: demonstrate the techno-economic viability of efficient capture, use and storage of CO/CO_2 streams from industrial installations, converting them into added value chemicals and materials; demonstrate cost efficient environmentally friendly technologies for capturing gas contaminants (e.g., use of waste heat in scrubbers, increased mass transport in intensified scrubbers, electrified systems with promising novel materials and equipment design) and develop fit for purpose gas purification approaches (e.g., advanced membranes, environmentally friendly absorbents and reliable catalysts for cleaning formulations, compression, drying, concentration, Pressure Swing Adsorption) while ensuring the maximum process efficiency including for downstream products; explore integration in existing systems; optimise the overall system by integrating advanced monitoring and control techniques based on digital technologies and perform socio-economic assessment.

- **Biomethane**: develop processes for capturing, refining and transforming methane from natural sources (for instance biogas), agriculture and landfills into chemicals. The focus should be on the development of biomethane at much higher percentages with integrated separation systems.

5.3. Clean, green and efficient production processes

The chemicals sector requires relatively high amounts of energy to produce primary or secondary materials of required purity for further processing. The chemicals sector is therefore depending on next generation of energy efficient technologies as well as on the integration of renewable energy and low-carbon energy vectors or fuels (e.g., green hydrogen) into its processes.

In many chemical processes, water plays an important role as raw material/feedstock or as process water, e.g., for cooling purposes. In the context of clean drinking water becoming one of the most challenging resources for the future of humankind, solutions for efficient water treatment technologies that prevent the contamination of the water resources and technologies to minimise water usage are urgently needed.

Research and innovation is needed in the following areas:

- **Energy efficiency and new sources**: develop highly energy efficient technologies addressing the most energy intensive parts of specific processes (e.g., reduce friction); improve tools and material efficiency, performance and durability; develop technologies to integrate renewable hydrogen into production routes for chemicals (including fuels).
- **Optimisation of thermal energy flows**: develop technologies to increase process energy efficiency by minimising and reusing thermal energy losses; enable lower temperature processes (e.g., via enzymes) to reduce energy demand; establish 'process integrated' solutions that offer better opportunities to increase the efficiency of high temperature installations e.g., heat exchangers or heat pumps.
- **Digitalisation of processes**: combine technologies for more efficient production with the digitalisation of processes enabling advanced automation and process control, predictive

maintenance and real-time process simulation as well as quality and emission control; enable cognitive plants; establish digital twins for the design and optimisation of processes.

- **Efficient use of feedstock**: develop new approaches (including industrial biotechnology) that will lead to higher resource efficiency e.g., solvent reduction and reuse, producing less low-value by-products and waste and enabling to cope with higher variability of feedstock. This includes technologies for process intensification, tighter processing controls, processes that adjust in real time to changes, solutions to ensure higher yields from complex and fluctuating raw material feeds such as more tolerant reactor concepts able to deal with feedstock variability or energy cost fluctuation and processes minimising waste generation.

- **Closed loop processes**: establish automated feedback, real time information for closed-loop control of the process/product parameters for the efficient control and stability of processes to optimise the use of resources and reduce product variability.

- **Increased efficiency of catalytic processes**: develop new catalysts, e.g., chemicals, materials, enzymatic and microbiological processes, to increase efficiency and selectivity of production of chemicals and materials.

- **Electrification of high temperature processes**: reduce CO_2 emissions by developing new electrified processes for high temperature heating systems, that can be powered with renewable electricity (e-cracker, e-furnace) capturing the full potential of renewable energy sources while ensuring process flexibility.

- **Chemical storage of renewable energy sources**: develop technologies to stabilise the system against fluctuating imbalances between the supply and demand of electricity.

- **Integrated water management**: develop integrated processes that will reduce water consumption and the amount of final industrial wastewater produced, such as concentrated metals or other inorganic sludges; apply digital technologies to reduce the intake by industry of drinking or purified water, manage water resources between industrial sites and reuse wastewater streams; develop closed loop systems where industrial wastewater is recovered, processed, and reused; establish findable, accessible, interoperable and reusable (FAIR) databases on water by combining data from industrial and public sources; develop methodologies to measure, monitor and remove pollutants, e.g., microplastics in urban wastewater; combine smart monitoring technology including, low-cost sensors and monitoring devices with artificial intelligence driven integrated system risk management models and decision support tools and technologies for water re-use in chemical industry.

6

Exposure

To prevent, control or eliminate the exposure of consumers, workers, vulnerable citizens and the environment to hazardous substances, it is important to understand the environmental fate and exposure pathways of such substances.

The EU manages different databases monitoring the occurrence of chemicals: e.g., the database for Substances of Concern In articles as such or in complex objects Products (SCIP)[40], which lists articles containing Substances of Very High Concern (SVHCs) that are placed on the EU market; the Information Platform for Chemical Monitoring (IPCHEM)[41], which reports on chemical monitoring data in humans, food and feed, air, water and products; and the European Pollutant Release and Transfer Register (E-PRTR)[42] database, which currently monitors and reports on 91 chemicals at the EU level.

However, significant gaps remain in our knowledge about the exposure of humans and the environment to which substances, in which quantity, from which sources and via what route[43]. Examples of exposure sources are environmental pollution, food, consumer products, domestic environments and workplaces. Exposures occur at different times and locations. Developments in our society – e.g., new consumption habits, new technologies and materials, new trades and urbanisation, demographic changes, and adaptation to climate change – are modifying exposure patterns. Some chemicals, such as endocrine disruptors or carcinogens, mutagens and reprotoxic (CMR) substances, can have a considerable impact on humans and on the environment, even with limited exposure. Other substances, such as persistent organic pollutants (POPs, e.g., PFAS) or persistent bioacumulative and toxic substances that cannot be easily degraded, remain in the environment and build up over time. There are novel emerging

40 SCIP database
41 IPCheM Portal
42 European Pollutant Release and Transfer Register
43 Fitness Check of the most relevant chemicals legislation (excluding REACH), as well as related aspects of legislation applied to downstream industries Fitness check chemicals legislation

pollutants (e.g., organophosphates, polymers, cyclic silicone-based chemicals, chlorinated paraffins) for which there are important information gaps. The so-called ‘More than One Constituent Substances’ (MOCS), including substances of ‘Unknown or Variable Composition or Biological substance (UVCBs), pose additional challenges. The cumulative exposure (total exposure to one chemical from all sources and routes) and combined chemical (mixture) exposures (exposure to more than one chemical from one or multiple exposure sources and routes) increase the complexity of understanding exposure impacts.

6.1. Exposure monitoring

Exposure monitoring (including biomonitoring, environmental monitoring and emission release measurements) provides data about levels of exposure and contributes to the validation of exposure models. Targeted analysis as well as non-targeted screening (NTS) can be used as a holistic approach to detect and identify emerging contaminants.

Research and innovation is needed in the following areas:

- **Monitoring strategies and campaigns**: develop strategies building on existing and planned monitoring schemes in EU legislation and reduce the time lag between the identification of a potential risk and its monitoring; extend monitoring schemes to measure a broader range of the chemical universe; integrate environmental and human (bio) monitoring to provide a holistic picture; extend the scope of one-off environmental monitoring (including in-situ monitoring) campaigns (such as watchlists) to determine reference background levels and combine with large scale targeted and NTS of the population; develop monitoring strategies based on the grouping of chemicals according to sources, uses, structural similarities, physico-chemical properties, modes of action and develop monitoring frameworks for exposure to mixtures; develop methods and collect data to better document consumer behaviours in relation to products (cosmetics, biocides, etc.); establish monitoring campaigns combining source related monitoring, geographical models on time and location, spatial information on production, sales, use, consumption and chemical composition; sustain EU-wide human-biomonitoring programmes and laboratory networks; establish quality assurance programmes for both target and non-target screening, including assessments on which level of certainty is sufficient for risk assessment.

- **Exposure pathways**: establish exposure pathways throughout the full life cycle of a chemical, i.e., between the environment and humans, including from consumer products and/or waste disposal; develop monitoring tools and methods to track the source and route of a chemical exposure as well as combined (multiple chemicals, multiple sources) and aggregated (same chemical, different sources) exposures, and be able to account for transformation products and substances unintentionally added during production processes.

- **Specimen banks**: establish and maintain banks with environmental and human samples to allow information to be collected on the retrospective temporal and spatial data trends of exposures to understand current exposures in their historical contexts.

- **Analytical methods and environmental sensors**: increase the sensitivity, speed, reliability and accessibility of routine analytical methods and develop low cost and easy to use monitoring equipment to allow for more frequent obligatory monitoring. The targeted demands are: real-time monitoring (using digital tools), the early identification of low-dose exposures, effect based/bioactivity-based monitoring, environmental omics fingerprinting or mapping, monitoring in complex matrices including those on diluted substances in particular for the identification and quantification of nanomaterials (or nanoforms) and polymers with low detection limits, dosing methods for difficult substances (e.g. polymers, poorly soluble, or volatile substances, microplastics), extraction of difficult substances from test systems, sensors to detect geometrical forms, aggregates and agglomerates of nanomaterials, sensors for multisource monitoring for the assessment of aggregated exposure, and protocols for mixture preparation (also addressing impurities), testing, monitoring and reporting.

- **Human biomonitoring tools**: validate innovative and cost-effective methods for assessing the exposure of humans to chemicals of concern e.g., low-cost personal sensor and wearable devices potentially equipped with geolocalisation systems; develop (metabol)omics-based biomarkers of both exposure and effect in non-invasive matrices (like urine, stool, sweat and exhaled breath) for large population screenings; develop new biomarkers for monitoring chemicals of upcoming concern and for circular economy subproducts and mixtures; link to registry/epidemiological studies and enable the comparison of exposure values and pathways for different population groups.

- **Non-target screening**: apply NTS for the detection of novel, emerging and unknown exposures and relate such exposures to known pollutants and their exposure trends/patterns; develop high-throughput, automated data processing and the exploitation of different datasets to enable the identification of the accurate compound and relationships between transformation products and parental chemicals; improve, harmonise and validate methods for generating (semi) quantitative data from NTS methods to integrate them into rapid risk assessment workflows; facilitate early warning and the identification of occurring mixtures; develop reference materials for chemicals and chemicals' sub-products and derivatives as well as compound libraries for NTS and encourage input from industry on their portfolios of substances.

- **Environmental fate characterisation**: elucidate the transformation of substances in the environment and their bioavailability, which includes approaches to measure and estimate degradability and co-formulants throughout the full life cycle of substances; develop methods that allow for a robust determination of a chemical parent's degradation half-life (DT50) to assess the persistence of substances that biodegrade less or more slowly than others in different media and improve mobility assessments; elucidate mode of action, grouping and behaviour of contaminants in sediment/soil and their potential release from sediment to water; understand how carriers and encapsulates influence the environmental fate and impact of ecosystems for a wide range of substances and mixtures. Specific targets are substitution candidates for POPs and active pharmaceutical ingredients, metals and organic compounds.

- **Exposure data and data analysis**: promote findable, accessible, interoperable and reusable (FAIR) exposure data that are accessible via established platforms and quality-checked spatial databases with improved spatial and temporal resolution for exposure modelling; establish open access toolboxes of methods (using artificial intelligence) for the reliable interpretation of monitoring data, which includes using robust statistical methods for outlier identification and handling of missing data (or data below the limit of detection) and tools using both chemical and biological knowledge to detect harmful pollutants in real-world samples.

6.2. Exposure models

An exposure model is a mathematical representation of an exposure scenario delivering a quantitative estimate. Advances in modelling and in quantification of their uncertainty are needed to be able to estimate future exposure levels, including long-term exposure, and safe concentration limits considering different environmental, economic, technological and social scenarios. Models should also help to prioritise substances for which further action is needed. Gender aspects and societal inequities need to be considered in all exposure models.

Research and innovation is needed in the following areas:

- **Environmental models**: ensure predictive environmental exposure models and real-life models that can support regulatory processes including quantifying uncertainty; develop models for source tracking using emission patterns when possible and including transformation patterns; update distribution and exposure models for substances in the environment to reflect how contaminants move between different environmental media and biota as a means of setting threshold values and environmental quality standards, in particular for environmentally persistent and mobile pollutants; develop models for different ecological niches so as to be able to consider different scenarios of chemical usage and chemical release from materials, products and waste as well as models that include multiple species; develop models for exposure and fate of nanomaterials, polymers and pharmaceuticals; increase interoperability of models and data to exploit the full potential offered by models.

- **Multiple exposure models**: develop exposure models allowing combined and aggregated exposure assessment for retro- and prospective exposure scenarios including modelling risks.

- **Early warning models**: establish early warning systems, including decision support for exposure reduction, using artificial intelligence based predictive eco-toxicology models that allow simulations of various scenarios linked with real-time monitoring sensor systems.

- **Human exposure models**: improve models for exposure of humans to chemicals from different sources via different exposure routes (e.g., inhalation, ingestion, skin); establish models linking external and internal exposure in humans and models considering mixture effects including co-exposure to other health stressors; develop real-life exposure models, and for entire life exposure, including exposure to multiple factors, with capacity of simulation at individual and population levels. Improve in vitro to in vivo extrapolation (IVIVE); develop Physiological Based PharmacoKinetic (PBPK) models and simulations to understand the concentration of chemicals at the points of toxicity in the human body; further develop organ-on-chip technologies for testing human exposure (including multiple exposure models).

- **Validation of models**: validate and standardise exposure models to foster their regulatory uptake and increase confidence in their usage; use biomonitoring data to refine generic models (‘reality-check’).

7

Hazard assessment

Many chemicals on the market are not sufficiently characterised for their presumed hazardous effects[3] and hazard assessment suffers from a blind spot as 'no evidence of an effect' does not equate to 'evidence of no effect'[44]. To speed up hazard assessments, cover more substances and species and move away from animal-based testing there is a need for a paradigm shift towards New Approach Methodologies (NAMs) to increase the use of the next generation of testing methods based on in vitro and in silico model systems. To enhance their applicability for regulatory decision-making, validation of these next generation testing methods as well as other new methods should be emphasised and OECD Test Guidelines updated as relevant.

It is important to develop methodologies based on high data treatment capacities and improved molecular modelling that will speed up our capacity to identify hazards and prioritize them for further assessment or risk management. Systems biology approaches may offer breakthrough possibilities to understand, model, and predict the interference of chemical substances with biological systems. Environmental hazard assessment should identify the effects of chemicals on organisms and related populations, communities, and ecosystems. Today, there is still lack of data for many species and relevant endpoints, allowing only for partial eco-toxicity assessments. A wider ecosystem approach is needed.

Research and innovation is needed in the following areas:

- **Integrated hazard assessment**: develop models to allow the integration of human health assessment and environmental assessment. Review assessment factors for extrapolating from ecotoxicity to human toxicity. Develop integrated protocols using effect-based methods for a wide range of relevant Mode of Action (MoA) in combination with non-targeted screening (NTS) followed by target analysis to identify toxic drivers of chemical mixtures occurring in the environment. Develop high throughput

44 Study for the strategy for a non-toxic environment of the 7th Environment Action Programme

methods facilitating the evaluation of many biological responses in a single test and/or increase the throughput of substances tested; develop integrated approaches to testing and assessment (IATA) combining methodological approaches such as Quantitative Structure-Activity Relationship (QSAR), read-across, in chemico, in silico, in vitro, ex vivo, in vivo or omics technologies to close the gap between the number of chemicals in use and the number assessed to date; link epidemiological, biomonitoring and toxicological studies and consider (population) vulnerability and genetic variation as well as non-biological contributors.

- **Mechanism based methods**: develop NAMs for assessing environmental hazard and bioaccumulation (e.g., for ionised chemicals and/or organo-metals) as well as biotransformation across organisms and species; advance in-vitro-to-in-vivo extrapolation (IVIVE); use NAMs to advance the read-across and grouping approaches of chemicals based on knowledge about their molecular mechanisms of action and resulting regulatory endpoints; use NAMs to support the uncertainty assessment of the link between upstream effects and downstream concerns and identify more suitable biomarkers of (early) effect and molecular key events (KE) biomarkers. Enhance quantitative Adverse Outcome Pathways (AOPs) and the time dimension linking different KE (life-course AOPs). Link KE biomarkers with AOPs to create a robust ontology for toxicities. Investigate morphologically triggered hazard properties.

- **Toxicokinetic data**: develop toxicokinetic data of substances (including mixtures, polymers, advanced materials and Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCBs)) including kinetic data of the biomarker of choice and conversion factors (i.e., what part of a dose is presented by the biomarker of choice).

- **(Eco)toxicity models and tests**: change from single (species) endpoints to study the impact on the entire ecosystem and develop advanced models and test methods to better understand the toxicity of chemicals and advanced materials across the entire ecosystem and to better prioritise species for which targeted testing is necessary; establish standard in-vitro and in vivo bioassays targeting new relevant endpoints in poorly addressed species (e.g., amphibians, reptiles, insects, arthropods and plants) beyond the traditional evaluation of carcinogenic, mutagenic and reprotoxic (CMR) risks and endocrine disruption (estrogenic, androgenic, thyroidal and steroidogenic (EATS)); develop complex models for several critical endpoints for genotoxicity, carcinogenicity, the immune system and inflammation, developmental toxicity, neurological and metabolic related diseases and the interaction of environmental chemicals with infectious agents; improve test systems for aquatic media and terrestrial in vitro tests; develop models for toxicity prediction both for acute short term exposure effects as well as for adverse outcomes due to long term exposures, for disease development, or generational effects; develop toxicokinetic/

toxicity models for estimating how much of an external exposure will reach target organs/tissues/cells at what rate and how will it be cleared; develop in chemico and in vitro virtual cell and multicell models and physiological and system biology models to assess interaction at molecular, cellular and tissue levels and to rapidly link exposure data to (human and environmental) health outcomes.

- **Substance specific**: develop robust toxicity assessment of micro/nano size matter (e.g., microplastics, nanomaterials) and investigate the long-range transport, uptake and toxicity for humans and other organisms; identify polymer-specific toxicities, characterise the determinants and review existing models for their adequacy to predict the 3D-molecular structures of polymers; study the effects of the (long-term) exposure to low levels of pharmaceuticals on humans via the environment; further investigate the toxicity of persistent, mobile and toxic (PMT) substances; develop standardised and validated test methods to investigate endocrine disruption in invertebrates as well as vertebrates; set-up in vitro approaches to gain mechanistic knowledge about endocrine disruption-induced adverse outcomes.

- **Mixtures**: study (eco)toxicological properties of (unintentional and intentional) mixtures and of the constituents that the mixtures contain; investigate the combined effects of chemicals on human health and environment with other external stressors (e.g., physical, climate change and social stressors) and genetics; identify key components of mixtures for relevant endpoints and for the qualification and quantification of substances interactions; perform proof-of-concept studies to demonstrate the likelihood of the synergistic effects of chemicals at low doses and related mechanisms; develop analytical methods to support Mixture Assessment Factors (MAFs) and the comparison between generic versus specific MAFs and further refinement of MAF values; strengthen mixture toxicity approaches for conventional and more complex materials of unknown or variable composition, e.g., for More than One Constituent Substances (MOCS).

- **Databases**: build an open database of synergistic and antagonistic interactions of substances to derive empirical mixture factors for different substance and interaction classes; develop databases on the mechanisms by which nanosized/micronized polymers may become bioavailable and/or hazardous for environmental species.

- **Data analysis**: use artificial intelligence to establish hazard mechanisms, including for mixtures; connect the hazard mechanisms with information on biotransformation pathways, toxicokinetics/bioaccumulation as well as species life history traits to understand the relevance of the predicted hazard mechanisms to affect populations; develop computational strategies to overcome data uncertainties related to in vitro tools and to replace data from in vivo and human clinical and epidemiological studies where possible
- **Decision support and guidelines**: establish approaches on how to consider uncertainties in the weight-of-evidence for the transformation assessment; develop new health-based limits values3, human biomonitoring-guidance values[45] and external health-based guidance values[46] for single substances as well as for mixtures; develop guidelines for UVCB substances based on key hazard markers or on molecule types in the substance; develop a library of testing strategies not only for the scientists, but also for other stakeholders (e.g., clinical, regulatory, and industrial).

45 Horizon 2020 European Joint Programme Cofund HBM4EU
46 Health-based guidance value

8

Risk assessment

In the EU, chemical regulations risk assessments are the basis for decision-making by risk managers who identify, quantity and manage the risks posed by chemicals. With increased knowledge about chemicals acquired over the years and the development of new technologies and new categories of chemicals, innovation in risk assessment paradigms is needed. It is essential to be able to prioritise substances according to the concern associated with their hazard and exposure brought about by their use.

The current risk assessment approaches are focussed on the use of selected species. Experience shows that ecosystems are very complex and that it is very difficult to evaluate, follow and react to protect all species with this approach. Therefore, it is necessary to better address the complexity of ecosystems and better consider biodiversity in environmental risk assessment.

To deal with the large number of chemicals on the market, it is necessary to move towards the use of grouping approaches and group-wise risk assessment based on structural similarities and similar mode of action as well as non-targeted monitoring strategies. Group-wise risk assessment will also better inform on the risks of combined exposures and contribute to preventing 'regrettable' substitutions[47] of chemicals.

Approaches for the combined exposure to different chemicals are under development, e.g., by the European Food Safety Authority (EFSA)[48]. Two reasonings can be used for mixture risk assessment. The first one is the mechanism-based mixture assessment using grouping of compounds with the same or distinct Mechanisms of Actions (MoA) or belonging to the same compound class. The second approach is based on real-life mixtures. The improvement of mixture risk assessment can be done (1) either by implementing a Mixture Assessment Factor (MAF) as an additional risk management measure in single substance risk assessment, (2) or via dedicated scientific approaches addressing specific mixtures.

47 ECHA Data to prevent regrettable substitution
48 EFSA Chemical Mixtures

Research and innovation is needed in the following areas:

- **Inclusion of exposure data**: develop tools allowing the use of observational data from epidemiology and cohort studies and human biomonitoring data in risk assessments and to link internal exposure to external exposure (and vice versa) for risk management decisions.

- **Grouping of chemicals**: develop efficient and mechanistic approaches, including the use of artificial intelligence, for grouping of chemicals including omics approaches supported by sufficient data on fate, bioaccumulation and (eco)toxicological properties before a risk assessment is being made, not only according to chemical class, but also considering chemicals acting on the same targets and chemicals that co-occur.

- **Improved methodologies and tools**: address performance, regulatory feasibility, legal compliance, protectiveness, data requirements and the reliability of the conclusions; compare New Approach Methodologies (NAMs) and traditional animal-based models to benchmark acceptable levels of uncertainty; develop and improve test guidelines for end points in risk assessment; address gaps in ex ante risk assessments for chemicals and materials in the early stages of development due to limited data availability; develop probabilistic risk assessment and models for cumulative risk assessment, combining information from different media, biota and humans.

- **Targeted approaches**: address contaminants of emerging concern, persistent, mobile and toxic substances (PMTs) and endocrine disruptors to improve coverage of vulnerable environmental compartments.

- **Information sharing**: develop tools and guidance for sharing information and data across different fields to support the 'one substance - one assessment' approach[3].

- **Risk mapping**: develop digital tools for interactive mapping of emissions and modelled exposure of all substances together with hazard profile to give information in which areas there is high contamination/pollution leading to high risk and where measures to protect mankind and environment must be taken.

- **Trust building and risk communication**: include social science and humanities research to help increase transparency, trustworthiness and trust (including trust drivers) in risk assessments and its role in protecting society; develop participatory research projects in response to citizens' growing concerns.

9

Decontamination and remediating pollution

As set out by the Zero Pollution Action Plan[49], pollution prevention should increasingly become the norm. Nevertheless, the significant pollution legacy of the past must also be addressed. There is an extensive body of environmental legislation protecting soil, water and air from hazardous substances. For example, the New Soil Strategy[50] provides the overarching framework to protect land and soil in the future. The Water Framework Directive[51] monitors pollutants in water with the aim to restore water quality and avoid future pollutions. Nevertheless, the significant pollution legacy of the past must also be addressed.

Many different events – e.g., the discharge of emissions, the use of harmful substances in industrial processes or inadequate waste disposal and accidents – lead to the pollution of the environment. Most of these cases also pose direct or indirect risks to humans. Different contaminants have different effects on human health and the environment, depending on their physico-chemical properties and their biological activity, alone and/or in mixture.

Local pollution is present in all EU countries. There are 2.8 million potentially polluted sites of which an estimated 14 % are expected to require remediation[52]. By 2018, 65 000 sites had been remediated in the EU. However, by far, most potentially contaminated sites are still left untouched. Only 44 % of Europe's surface waters achieve good or high ecological status, partly because of pollution. Around 25 % of Europe's groundwater areas do not have a 'good chemical status'[53].

49 Zero Pollution Action Plan
50 Roadmap - New Soil Strategy - healthy soil for a healthy life.
51 EU Water Framework Directive
52 Status of local soil contamination in Europe
53 Ensuring clean waters for people and nature.

The contamination problem is mainly caused by synthetic chemicals and heavy metals originating from human activities both on land and at sea[54].

Research and innovation is needed in the following areas:

- **Risk analysis and management of existing pollution**: establish baseline data on natural resource and ecosystem resilience and develop processes that anticipate risks of existing pollution of air, water (surface, groundwater and marine) and soil (including sediments); develop decision tools considering sustainability challenges and the difficulties of data gaps and site-specific conditions (e.g., geography, geology, land/water use, vicinity of vulnerable receptors); develop standardised toolboxes of instruments for risk assessments.

- **Monitoring pollution**: develop high-resolution methods to measure persistent and mobile chemicals in different media (soil/water/air/sediment/waste) as well as high resolution digital models of contaminant mobility and (geo)chemistry in and between different media (soil/water/air/sediment); collect monitoring data to establish baselines and show the effectiveness of remediation activities at the intervention level.

- **Remediation strategies**: establish remediation strategies based on risk analysis (e.g., for the remediation of PFAS contamination in groundwater and soil) and sustainability requirements (e.g., minimising environmental and carbon footprints, maximising resource efficiency); ensure participatory processes creating local acceptances and when possible, contributions to interventions; define efficient protection measures for workers involved in decontamination and remediation.

- **Decontamination and treatment techniques**: develop cost-and-time effective techniques, including bio-remediation techniques, to remove contamination from different media with a focus on persistent and mobile chemicals (like PFAS) or selected anthropogenic (nano)materials; establish different techniques and advanced materials for remediation, e.g., filters, chemical degradation catalysers, to be able to address the full range of magnitude of sites and time and cost constraints; produce guidance for sustainable remediation methods.

- **Storage of contaminated materials**: enable safe deposition or capping of contaminated materials, including considerations for how to adapt to increased frequency of natural disasters.

- **Cost-benefit balance**: develop methods for sustainability analysis to compare the effectiveness and needed resources for different remediation approaches.

54 Contaminants in Europe's seas Moving towards a clean, non-toxic marine environment.

10

Monitoring implementation

A methodology for monitoring funding deployed under Horizon Europe for research and innovation (R&I) to achieve sustainable chemicals and materials will be developed and made publicly available. This is a first step in monitoring the successful implementation of the Strategic Research and Innovation Plan (SRIP) towards meeting its objectives and assess the impact of the SRIP on the R&I landscape.

The developed R&I indicator will include the number of relevant projects funded under Horizon Europe that address the challenges identified in the SRIP and their allocated budgets. The indicator will be updated at regular intervals, triggered by the adoption of the work programmes that set out funding opportunities for dedicated periods.

This R&I indicator will not only support Horizon Europe but will also provide added value for the monitoring of research investments relevant for achieving the objectives of the Chemical Strategy for Sustainability (CSS). In particular, it can provide a fact base to support the assessment of progress in specific domains identified in the framework of CSS indicators[55].

The methodology developed here will be available for application by other funding programmes at both the EU[56] and national levels to monitor their investments. Feedback from other programmes is welcomed to allow an overall reporting on R&I investments made in line with the SRIP.

55 Implementation of the Chemicals Strategy
56 Funding for the chemicals strategy

11 Conclusions

This Strategic Research and Innovation Plan (SRIP) intends to support the development of safe and sustainable chemicals and materials by proposing a holistic overview of R&I needs, collected through consultations with stakeholders, across the life cycles of chemicals and materials. By highlighting the key R&I needs for chemicals and materials across their lifecycle this SRIP represents a necessary step towards better addressing the interdependencies between safety, circularity, and the overarching sustainability goals. It is also an opportunity to support a more transparent communication among all relevant actors on joint future R&I priorities proposed by the wider community: from academia to SMEs, largescale industry, regulators and policy makers. Together with the future monitoring system the aim is to guide research and innovation funders in their decisions on investments across EU, national and private funding programmes.

The Commission will refer to this SRIP in the Horizon Europe work programme as an overarching strategy to which Horizon Europe contributes as a means of addressing the identified challenges.

The Commission invites research and innovation funders across EU, national and private funding programmes as well as researchers and innovators to support this strategy and to contribute to its implementation.

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The EU Open Data Portal (**http://data.europa.eu/euodp/en**) provides access to datasets from the EU. Data can be downloaded and reused for free, for both commercial and non-commercial purposes.

The Chemicals Strategy for Sustainability (CSS) is part of the EU's zero pollution ambition, which is a key commitment of the European Green Deal. The Strategy aims to better protect citizens and the environment and to boost innovation for safe and sustainable chemicals. To this end, it announces a Strategic Research and Innovation Agenda in 2022. The current Strategic Research and Innovation Plan (SRIP) delivers on this announcement and highlights current research and innovation (R&I) areas crucial for accelerating the transition to chemicals and materials that are safe and sustainable. The aim of the SRIP is to guide R&I funders in their decisions on investments across EU, national and private funding programmes. It is also an opportunity for a more transparent communication among all relevant actors on joint R&I priorities proposed by the wider community: from academia to SMEs, large-scale industry, regulators and policymakers.

Research and Innovation policy

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