# Safe-by-design for materials and chemicals: Towards an innovation programme in Horizon Europe

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# SAFE-BY-DESIGN FOR MATERIALS AND CHEMICALS

## Towards an innovation programme in Horizon Europe

**NON-PAPER**

**FINAL VERSION**

# SAFE-BY-DESIGN FOR MATERIALS AND CHEMICALS

## Towards an innovation programme in Horizon Europe

This non-paper is the result of the work of an informal working group of experts from government, academia and industry, composed of the following members:


| | |
|---|---|
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The document does not necessarily represent the official views of the organisations involved but serves to support discussions in the preparation of Horizon Europe.


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# EXECUTIVE SUMMARY

**Objectives and background**

Chemicals are essential to perform a wide variety of functions in society and contribute significantly to our well-being. They play a substantial role to create added value along nearly all value chains across industrial sectors. With a workforce of 3.3 million persons (including pharmaceuticals and rubber and plastics) and sales of € 542 billion (2017), the chemicals industry is one of the biggest industrial sectors in the EU and an important source of direct and indirect employment.[1]
In view of the worldwide growth in chemicals and chemical-intensive products, improvement of the safety of chemicals, materials and products, also within the context of circular economy, will contribute to attaining several Sustainable Development Goals (SDGs). Studies suggest that damage to human health and the environment due to hazardous chemicals - or potential gains of avoiding them - are in the order of tens or even hundreds of billions of euros per year for the EU.[2,3]

The concept of safe-by-design aims to prevent negative impacts on human health and the environment, by considering safety aspects early in the design process of chemicals, materials and products. There are several reasons to place more emphasis on innovation for safe-by-design. It complements regulations as a more efficient way of increasing safety, as risks are prevented rather than managed. It also enables the transition towards a circular economy, which requires inherently safer materials that maintain their quality through multiple material cycles, including repair, reuse and recycling.

While the starting point of safe-by-design is to minimise toxicity (including persistency and bio-accumulation, and including products of incomplete degradation/mineralization), it is clear that global challenges related to pollution, climate change and environmental degradation can only be tackled with products that are sustainable in a wider sense, including aspects such as energy and resource efficiency, and emission and exposure minimisation. Safe-by-design requires a full life cycle perspective and needs to be combined with overall sustainability improvements, also to avoid the shifting of negative consequences across life cycle stages and impact categories.

Safe-by-design not only helps to prevent hazards from newly invented chemicals, processes and materials but is also an approach to redesign existing applications where chemicals give rise to environmental and health concerns. In several key applications (water and dirt repellency, fire safety, preservation, solvents etc.), the challenge to find safer and effective alternatives has been very persistent and ongoing. Although many alternatives have been introduced to well-known hazardous chemicals, substitution often remains limited to structural analogues. For several chemical groups, evolving knowledge has led to concerns about these analogues as well, with a risk of regrettable substitution. Hence, there is a need to seek for safe-by-design products, services and materials, whilst accounting for their full life cycles.

In the global transition to a safe and circular economy, the EU can play a leading role by developing innovative, safer and sustainable materials, chemicals, products and services. EU innovation policy, as a complement to chemicals policy, could stimulate the development and adoption of such innovations. *This non-paper suggests the main topics for an innovation programme, in Horizon Europe or other European programmes, that could accelerate the design, development and adoption of safer*

[1] CEFIC (2018), Facts and figures of the European Chemical Industry.
[2] UNEP (2019), Global Chemicals Outlook, synthesis report, p.31-32.
[3] Gretta Goldenman, Meena Fernandes, Michael Holland, Tugce Tugran, Amanda Nordin, Cindy Schoumacher and Alicia McNeill (2019). The cost of inaction - A socioeconomic analysis of environmental and health impacts linked to exposure to PFAS.

*alternatives to new and existing applications (materials, chemicals, products and services) where safety hazards (may) arise.*

This non-paper is the result of the work of an informal working group of experts from government, academia and industry.[4] *The document does not necessarily represent the official views of the organisations involved but serves to support discussions in the preparation of Horizon Europe.* The document paper builds on the Safe Chemicals Innovation Agenda (SCIA) that was drafted by Wood and CSES[5], in consultation with stakeholders, and commissioned by the Netherlands' Ministry of Infrastructure and Water Management. The working group has consulted additional experts and stakeholders during the preparation of this document (Annex 1). Part of this consultation was a workshop on 16 May 2019 organised by SusChem, the European Technology Platform for Sustainable Chemistry.

**Relevance and impact of a safe-by-design programme**

A programme for safe-by-design that brings about better safety profiles of products, materials, processes and services would contribute to many, if not most, of the Sustainable Development Goals. The relevant SDGs include: sustainable agriculture (SDG 2); healthy lives and well-being (SDG 3); clean water and sanitation (SDG 6); decent work and economic growth (SDG 8); resilient infrastructure, inclusive and sustainable industrialisation and innovation (SDG 9); sustainable cities and communities (SDG 11); responsible consumption and production (SDG 12); climate change (SDG 13); life below water (SDG 14); and life on land (SDG 15).[6]

More specific areas of impact are the following:

- Human health: avoiding illness and associated reduced quality of life, loss of productivity and health care costs and premature mortality.
- Ecosystems in Europe: reduced exposure due to contamination of water, air and soil, and improvement of the value of ecosystem services, preservation of ecosystems.
- Circular economy: safe-by-design enables easier reuse, repair and recycling of materials by using substances that are compatible with new lifecycles.
- Avoidance of future costs for business: avoidance of regrettable substitution, which will limit costs to comply with (future) legislation and productivity loss at the workplace.[7]
- Boosting innovation and competitive advantages, related to the value of sustainability aspects for consumers and investors.
- Increased policy coherence and efficiency: a programme with a consistent approach towards different chemical applications is more efficient compared to isolated projects.

**Potential areas of funding**

There are the following three proposed funding areas for a Horizon Europe programme (see figure 0.1):

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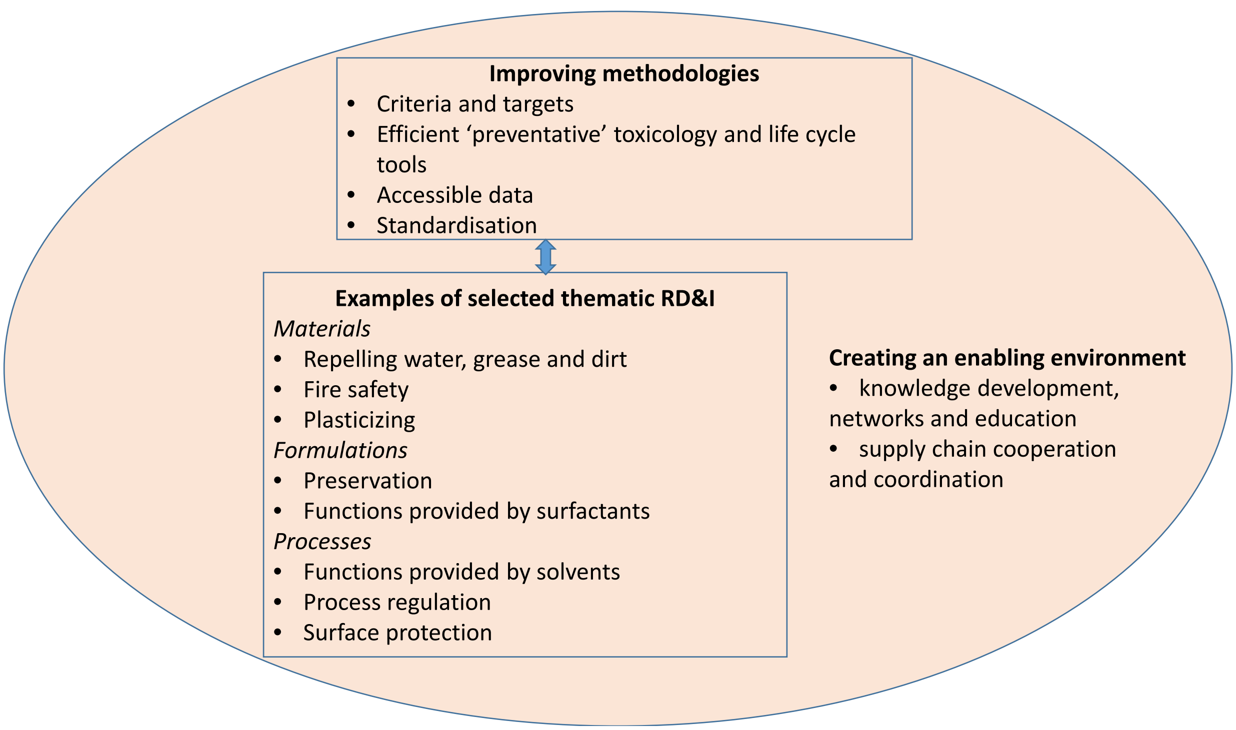
[4] The Dutch Ministry of Infrastructure and Water Management, the European Environmental Agency, the European Chemicals Agency, BioNanoNet, the Technical University of Denmark, SusChem ETP.
[5] Centre for Strategy and Evaluation Services.
[6] As part of SDG 3 (Ensure healthy lives and promote well-being for all at all ages), target 3.9 is: By 2030, substantially reduce the number of deaths and illnesses from hazardous chemicals and air, water and soil pollution and contamination. Under SDG 12 (Ensure sustainable consumption and production patterns), target 12.4 is: By 2020, achieve the environmentally sound management of chemicals and all wastes throughout their life cycle, in accordance with agreed international frameworks, and significantly reduce their release to air, water and soil in order to minimise their adverse impacts on human health and the environment.
[7] UNEP (2019), Global Chemicals Outlook, p. 164-175.

- Developing or improving methodologies: reliable and suitable methodologies for safe (re)design of chemicals and materials have to be (further) developed to ensure that toxicity and other lifecycle considerations (including circularity) are integrated into design processes.
- Addressing thematic Research, Development and Innovation (RD&I) needs: RD&I is needed to overcome technical and scientific challenges in areas where it has been difficult to find safer alternatives. Such RD&I should be based on a functional approach, which means that the focus is on the function performed by chemicals (e.g. water and dirt repellency, fire safety, preservation etc.) rather than chemical structure as such. Methodologies for safe-by-design need to be applied to (re)design and assess solutions for different applications, avoiding the use of hazardous chemicals whilst improving by design the lifecycle safety and sustainability profile. This can be done at potentially very different levels (chemical, material, product, process, business models), including non-chemical solutions.[8] Thus far, most research has been conducted at chemical substances level (chemical-by-chemical substitution). Innovating on material structures, product and process improvements can be given more emphasis, as part of the functional substitution concept. This also means that assessments of toxicology and other sustainability aspects need to cover materials, products and processes as a whole. This broader perspective brings about the involvement of other disciplines and stakeholders across value chains and sectors.
- Creating an enabling environment: Safe-by-design - as a new interdisciplinary approach - needs to be set up, to develop terminology, methods and tools. Knowledge exchange, education/skills and supply chain cooperation are important aspects of an enabling environment. Awareness raising is paramount because safe-by-design involves a change in mind-set in businesses, including at the executive positions. Activities not primarily focused on research but aimed at networking, awareness raising and education can also be part of EU innovation programmes.

*Figure 0.1 Basic elements of a European safe-by-design programme*




[8] the term 'non-chemical solutions' may not be fully accurate, since alternative materials or technologies will also involve chemicals. However, this term is meant to also refer to alternatives where the function previously performed by hazardous chemicals/additives could now be provided by innovation at the levels of materials, products, services or processes.

Table 0.1 summarises the suggested research, development and innovation focus areas.

*Table 0.1 Suggested research, development and innovation focus areas*

| | |
|---|---|
| | ***Improving methodologies*** |
| **Criteria and targets** | • Harmonised and validated criteria and science-based targets for safety and sustainability for the whole life cycle of service/product/material/chemical, also enabling the transition to circular economy |
| **Efficient 'preventative' toxicology and life cycle tools** | • Methods and digital tools for integrating knowledge of toxicity into early design and to evaluate sustainability impacts throughout the lifecycle |
| **Accessible data** | • Make data available (criteria for Findable, Accessible, Interoperable and Reusable data in research calls, add data to open access databases) |
| **Standardisation** | • Involve standardisation bodies to ensure optimum use of standards and development of new standards (data, methods, tools) |
| | ***Performing thematic RD&I*** |
| | *Materials* |
| **Repelling water, grease and dirt** | • New materials design approaches to achieve inherent repellence performance function (e.g. reverse osmosis membranes for fabrics)<br>• Innovative repellent materials using alternative chemicals with positive scores on safety and ability to mineralise |
| **Fire safety** | • Innovative materials with inherently flame-resistant function<br>• Materials design to reduce additive exposure/leaching to the environment (intermediate solution) |
| **Plasticizing** | • Innovative materials with the same functionality (flexibility, durability) in the absence of hazardous additives (in final product and production process)<br>• Novel and sustainable material/chemical combinations with plasticizing function |
| | *Formulations* |
| **Preservation** | • Preservation systems based on alternative mechanisms (e.g. heat treatment, electrostatic spraying, physical and chemical treatment combinations etc.)<br>• Mechanisms of antimicrobial activity with new chemical-material combinations (raw materials combinations & design approaches) |
| **Functions provided by surfactants** | • Sustainable production of alternative raw materials that combine safety and life-cycle sustainability performance<br>• Formulation redesign with alternative surfactants whilst understanding complex behavior of new molecules in mixtures/formulations and implications of production scaling up |
| | *Processes* |
| **Functions provided by solvents** | • Innovative materials with reduced surface treatment requirements<br>• Process innovations to avoid hazardous solvents in production processes<br>• Alternative formulations/chemicals for process solvents |
| **Process regulation** | • Innovative foams and resins |
| **Surface protection** | • Alternative materials that are inherently resistant to corrosion or fouling<br>• Development of new techniques for surface treatment |
| | ***Creating an enabling environment*** |
| **Knowledge development, networks and education** | • Network building as objective or condition in funded projects<br>• Extracurricular activities, challenges and competitions, bootcamps, educational networks as start of a process of internalizing safe-by-design in education and skills development<br>• Landscape analysis of existing disciplines, networks and organisations |
| **Supply chain cooperation and need for coordination** | • Scoping phase with stakeholders before technical research to:<br>1) analyse context of the innovation (potential barriers)<br>2) identify user needs and performance criteria<br>3) identify appropriate levels of research (material, process, product, chemical)<br>• Coordinating body with research programme to oversee learning and innovation processes, and to make information available<br>• Data and knowledge sharing platforms across value chains and different sectors |

The thematic RD&I areas have been identified in the consultation process explained above (preparation of the Safe Chemicals Innovation Agenda, consultation of experts, SusChem ETP workshop) and are thus based on expert judgement, qualitatively using criteria such as relevance for human health and the environment, the presence of scientific and technical challenges, and economic importance. However, it should be noted that the approach – in particular relating to methodologies and the enabling environment – is applicable to all functions performed by chemicals. Furthermore, additional themes (not elaborated in this non-paper) could be considered, including pharmaceuticals, pesticides, fertilisers and heavy metals used for energy storage (batteries). In the preparation of this non-paper, stakeholders also suggested additional functionalities:

- materials: UV-stabilisation and anti-oxidation for materials, in particular related to paints and coatings;
- formulations: stabilization (e.g. foams, emulsions, suspensions), colorants (dyes or pigments) and mechanical abrasives;
- process applications: preservation (e.g. process fluids), additives (e.g. softeners) and fuels.

**Next steps**

The working group recommends to consider the options for a safe-by-design programme in Horizon Europe and possibly other European programmes, such as LIFE. Within Horizon Europe, there are opportunities in Pillar II (Global Challenges and European Industrial Competitiveness), in particular in the clusters ‘Health’, ‘Digital, Industry and Space’ and ‘Food, Bio-economy, Natural Resources, Agriculture and Environment’.[9] In fact, the European Commission already suggested safe chemical design as potential subject within these clusters.[10] There are also potential links with the proposed Partnership on Chemicals Risk Assessment and with several Missions, which could be further explored.

[9] Horizon Europe framework programme for research and innovation 2021–2027. 2018/0224 (COD) Text adopted by Parliament, 1st reading/single reading (17 April 2019).
[10] European Commission (2018), ANNEXES to the Proposal for a DECISION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL on establishing the specific programme implementing Horizon Europe – the Framework Programme for Research and Innovation. P. 35 and 51/52.

# 1 INTRODUCTION

## 1.1 Rationale and objectives

In modern society, chemicals play an important role in the process of creating the enormous array of products that we use and from which we derive a large part of our well-being. Some chemicals however, may have negative impacts as well. Despite major progress in environmental policies, hazardous chemicals can provoke substantial negative effects to health and the environment.[11] Hence, there is a need to seek for new products, services and materials that - in their full lifecycles - do not rely on or release hazardous substances.

The concept of safe-by-design presents an approach to help prevent these negative impacts by considering safety aspects early in the design process of chemicals, materials, products and services. The concept has gained prominence in several fields, such as nanomaterials and biotechnology, and has been addressed in projects within Horizon 2020 centred on nanosafety. It is in line with the 7th Environment Action Programme[12], which mandated the European Commission to develop by 2018 "a Union strategy for a non-toxic environment that is conducive to innovation and the development of sustainable substitutes including non-chemical solutions."

While the starting point of safe-by-design is to minimise toxicity (including persistency and bio-accumulation), it is clear that global challenges related to pollution, climate change and environmental degradation can only be tackled with products that are sustainable in a wider sense, including aspects such as energy and resource efficiency, and emission and exposure minimisation. Safe-by-design requires a full life cycle perspective and needs to be combined with overall sustainability improvements, also to avoid the shifting of negative consequences across life cycle stages and impact categories.

One reason to put more emphasis on innovation for safe-by-design is that it complements regulations as a more efficient way of increasing safety. Regulations can restrict certain hazardous substances, but are usually only established after it is clear that these chemicals have harmful properties. In such cases, these chemicals are restricted in new products and processes, while they remain present in older products and/or – in the case of persistent and bio-accumulative substances - in the environment. Furthermore, regulations often provoke only shallow substitution by structural analogues, which can be used as a drop-in without the need for substantial redesign of the production process, materials, products or services. Initially there is usually less information about the hazards of these analogues. Additional information that may become available over time could later trigger regulations for these substances. This mechanism or regrettable substitution is a form of maladaptation to societal concerns that hinders fundamental progress towards the non-toxic environment, and impedes the competitiveness of European industry.[13] An innovation approach for safe-by-design, as a complement to regulations, could address these concerns.

A second reason is the transition towards a circular economy. This transition reinforces the need for inherently safer materials that maintain their quality through multiple material cycles, which may include repair, reuse and recycling. However, when a substance first enters the market, it is

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[11] European Commission (2017), Study for the strategy for a non-toxic environment of the 7$^{th}$ Environment Action Programme. UNEP (2019), Global Chemicals Outlook, From Legacies to Innovative Solutions. Synthesis Report.
[12] Decision No 1386/2013/EU of the European Parliament and of the Council of 20 November 2013 on a General Union Environment Action Programme to 2020 'Living well, within the limits of our planet'.
[13] Milieu Ltd, Ökopol, RPA and RIVM (August 2017), Study for the strategy for a non-toxic environment of the 7$^{th}$ Environment Action Programme. Tickner and Jacobs (2016). Needs and opportunities to enhance substitution efforts within the context of REACH.

challenging to anticipate exposures associated with future uses in subsequent material cycles. Chemicals that have initially not been classified as hazardous (or for which no risk management regulatory action was deemed necessary) may later be found to be substances of concern. This calls for products that can be fully deconstructed to monomaterials with a low hazard profile, or for additives that can be relatively easily removed from materials.[14] There are also chemicals in materials or products that cannot (easily) be recycled as they enter the environment via open applications, waste water or abrasion (e.g. pesticides, pharmaceuticals, laundry detergents, cosmetics, abrasion of paint or tires) and this can be an additional motive to search for safer alternatives.

The dynamics of innovation can be considered a third consideration to take more action on safe-by-design. Between 2000 and 2017, the global chemical industry's production capacity (excluding pharmaceuticals) almost doubled, from about 1.2 to 2.3 billion tonnes.[15] The total number of industrial chemicals in commerce globally has been estimated at 40.000 to 60.000, with 6.000 of these chemicals accounting for more than 99 per cent of the total volume.[16] The number of chemicals on the market is exceeded by a larger – and growing – number of chemical-intensive products such as computers, mobile phones, furniture, and personal care products.[17] Legislation alone cannot keep up with the growth in the number of new chemicals and chemical-intensive applications. Global developments in the field of energy, such as electrification and the rise of renewable chemicals, will result in different industrial processes with possibly new chemicals and materials. In the fields of nanomaterials and biotechnology, the dynamics of innovation are even more important drivers for safe-by-design. In the field of chemicals and materials, the challenge is in fact twofold: to prevent hazards from novel chemicals, processes and materials and to redesign existing applications where safety and sustainability hazards arise.

The above elements give rise to the question how EU research, development & innovation can complement chemicals policy, and stimulate the development and use of materials, chemicals, products and services that are safe-by-design. More specifically, the authors recommend including a dedicated programme in Horizon Europe[18] and/or possibly other European programmes (such as LIFE) to address the major gaps in knowledge and development in this field. The impacts of such a programme are potentially large (see text box).

**The aim of this non-paper is to suggest the main topics for an innovation programme, in Horizon Europe and/or other European programmes, that could accelerate the design, development and adoption of safer alternatives to new and existing applications where safety hazards (may) arise.**

[14] See OECD (2019), Workshop on Approaches to Support Substitution and Alternatives Assessment.
[15] UNEP (2019), Global Chemicals Outlook, From Legacies to Innovative Solutions. Synthesis Report, p. 17.
[16] UNEP (2019), Global Chemicals Outlook, From Legacies to Innovative Solutions. Synthesis Report, p. 4.
[17] UNEP (2019), Global Chemicals Outlook, From Legacies to Innovative Solutions. Synthesis Report, p. 4.
[18] Proposal for a REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL establishing Horizon Europe, 7942/19.

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**Text box** **Impacts of a safe-by-design programme in Horizon Europe**

A programme for safe-by-design that brings about better safety profiles of products, materials, processes and services would contribute to many, if not most, of the Sustainable Development Goals. The relevant SDGs include: sustainable agriculture (SDG 2); healthy lives and well-being (SDG 3); clean water and sanitation (SDG 6); decent work and economic growth (SDG 8); resilient infrastructure, inclusive and sustainable industrialisation and innovation (SDG 9); sustainable cities and communities (SDG 11); responsible consumption and production (SDG 12); climate change (SDG 13); life below water (SDG 14); and life on land (SDG 15).[19]

More specific areas of impact are the following:

- Human health: avoiding illness and associated reduced quality of life, loss of productivity and health care costs and premature death.
- Ecosystems in Europe: reduced exposure due to contamination of water, air and soil, and improvement of the value of ecosystem services, preservation of ecosystems.
- Circular economy: safe-by-design enables easier reuse, repair and recycling by using substances that are compatible with new lifecycles.
- Avoidance of future costs for business: avoidance of regrettable substitution, which will limit costs to comply with (future) legislation and productivity loss at the workplace.[20]
- Boosting innovation and competitive advantages, related to the value of sustainability aspects for consumers and investors.
- Increased policy coherence and efficiency: a programme with a consistent approach towards different chemical applications is more efficient compared to isolated projects.

A robust socio-economic analysis that covers all impacts is currently not possible (no system in place to track impacts, multiple causal factors, lack of data etc.). However, studies on specific issues suggest that damage due to hazardous chemicals - or potential gains of avoiding them - are in the order of tens or even hundreds of billions of euros per year. One study on neurobehavioral deficits caused by endocrine disruptors estimated the costs in the EU at over 150 billion euros per year.[21] Another study that included other effects of endocrine disruptors estimated costs at 163 billion euros per year, over 1 per cent of the EU's GDP.[22] A 2017 study conservatively estimated the cumulative benefits of chemicals legislation in the EU to be "in the high tens of billion Euro per year".[23] A recent study estimated yearly costs due to exposure to PFAS and C4-14 non-polymer fluoro-surfactants in the order of € 52 to 84 billion in the EEA countries, for those health impacts for which risk data are available.[24] At global level, damage to the environment by chemicals has been estimated at several percentage points of global gross domestic product.[25] [26]

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[19] As part of SDG 3 (Ensure healthy lives and promote well-being for all at all ages), target 3.9 is: By 2030, substantially reduce the number of deaths and illnesses from hazardous chemicals and air, water and soil pollution and contamination. Under SDG 12 (Ensure sustainable consumption and production patterns), target 12.4 is: By 2020, achieve the environmentally sound management of chemicals and all wastes throughout their life cycle, in accordance with agreed international frameworks, and significantly reduce their release to air, water and soil in order to minimise their adverse impacts on human health and the environment.

[20] UNEP (2019), Global Chemicals Outlook, p. 164-175.

[21] Bellanger, M., Demeneix, B., Grandjean, P., Zoeller, R.T. and Trasande, L. (2015). Neurobehavioral deficits, diseases, and associated costs of exposure to endocrine-disrupting chemicals in the European Union. *Journal of Clinical Endocrinology & Metabolism*. 100(4), 1256-1266.

[22] Trasande, L., Zoeller, R.T., Hass, U., Kortenkamp, A., Grandjean, P., Myers, J.P., DiGangi, J., Hunt, P.M., Rudel, R., Sathyanarayana, S., Bellanger, M., Hauser, R., Legler, J., Skakkebaek, N.E. and Heindel, J.J. (2016b). Burden of disease and costs of exposure to endocrine disrupting chemicals in the European Union: an updated analysis. *Andrology*. 4(4), 565-572.

[23] Amec Foster Wheeler [now the Wood Group], Brunel University, Economics for the Environment Consultancy and Peter Fisk Associates (2017). *Study on the Cumulative Health and Environmental Benefits of Chemical Legislation*.

[24] Gretta Goldenman, Meena Fernandes, Michael Holland, Tugce Tugran, Amanda Nordin, Cindy Schoumacher and Alicia McNeill (2019). The cost of inaction - A socioeconomic analysis of environmental and health impacts linked to exposure to PFAS.

[25] Grandjean, P. and Bellanger, M. (2017). Calculation of the disease burden associated with environmental chemical exposures: application of toxicological information in health economic estimation. *Environmental Health* 16(123), 1-13.

[26] For an overview of several studies: UNEP (2019), Global Chemicals Outlook, p. 170-175.

## 1.2 Preparation of this non-paper

This non-paper is the result of the work of an informal working group of experts with a background in government, academia, and industry.[27] The working group has consulted additional experts and stakeholders during the preparation of this document. This includes industry representatives, NGOs and Member States (see Annex 1).

The non-paper builds on the Safe Chemicals Innovation Agenda (SCIA) that was drafted by Wood and CSES[28] and commissioned by the Netherlands' Ministry of Infrastructure and Water Management. This SCIA was based on a desk study and interviews with experts and stakeholders, and was tested during an international workshop in Amsterdam in March 2018. The working group supplemented the SCIA with additional insights based on its own expertise, additional consultations, and new publications. In addition, a workshop organised by SusChem (SusChem SIRA workshop, May 16-17 2019) was used to gain additional input from stakeholders.

## 1.3 Structure of the non-paper

The mission of a program would be to accelerate the design, development and adoption of safe-by-design alternatives to improve the safety profile of chemicals, materials, processes and products, accounting for the full lifecycle (figure 1.1).

Three conditions follow from this overall mission:

- essential performance needs are fulfilled (e.g. corrosion protection, water and dirt repellency of materials, fire protection etc.);
- safety and sustainability are improved;
- actors acknowledge and play their role for safety.

Safe-by-Design is a specific approach to achieve these objectives, complementary to regulations. It seeks to include safety as a design requirement at the earliest stages of product and process development to prevent possible hazards for human health and the environment.

Five essential elements of safe-by-design contribute to the aims:

- A ***functional approach*** is key. To develop alternatives to applications with hazardous substances we need innovation that starts from considering the function(s) that the substance fulfills, including alternative ways to realize it or optimizing the performance requirements to the justified level. The functional approach broadens the perspective to include not just chemical-by-chemical replacement, but also solutions at the levels of materials, products, processes and business models, including non-chemical solutions.[8] Thus far, most research has focused on chemical-by-chemical substitution. Innovating on these higher levels can be given more emphasis.
- ***Minimising toxicity*** is the starting point. Health and environmental hazards such as carcinogenicity, mutagenicity, reprotoxicity, PBT properties (persistence, bioaccumulation, toxic), sensitizing effects, endocrine disruption etc. should be minimised, with a targeted and selective function of any applied compounds. This includes not only parent compounds but also potential products of incomplete degradation/mineralisation. Designs that allow mineralization of substances (i.e. degradation to carbon dioxide, water and inorganic salts) can be part of a solution to avoid persistence and bio-accumulation.

[27] The Dutch Ministry of Infrastructure and Water Management, the European Environmental Agency, the European Chemicals Agency, BioNanoNet, the Technical University of Denmark, SusChem ETP. Individuals from these organisations provided their expert input to the work, however this non-paper does not necessarily represent the official views of the organisations they belong to.
[28] Centre for Strategy and Evaluation Services.

- In addition to toxicity, the overall environmental and societal impact as well as other sustainability criteria should be considered. Safe-by-design requires a ***full life cycle perspective*** and needs to be combined with overall sustainability improvements in order to avoid the shifting of negative consequences across life cycle stages (e.g. from reduced consumer exposure during product use to increased environmental exposure during manufacturing) and impact categories (e.g. from reduced material consumption to iincreased exposure from cross-contamination associated with material recycling). In fact, positive impacts on other sustainability aspects are aimed for, such as those related to circularity or prolonged life spans (resources of materials and energy), but also emissions to air and water must be considered. Safety is also broader than toxicity, including physical safety, microbiological safety and biosafety. Taking a full life cycle perspective does not imply that all aspects can be traded against each other (e.g. to allow for a bad score on toxicity because of benefits for climate change). A full life cycle perspective also means that safe-by-design can be an aspect of ***circular design.*** Circular design aims to circle resources in loops and minimise waste. Safe-by-design implies avoidance of chemicals that hamper such loops. However, circularity is not by definition the most sustainable option, since it also comes at economic and environmental costs (e.g. energy use), and prolonged lifetimes (of materials and products) can be overall more sustainable than multiple life stages.
- It requires a ***multidisciplinary approach***. Fundamental innovation going beyond drop-in replacement requires integrations of scientific disciplines such as materials (circular) design and performance, chemistry, toxicology, sustainability assessment, product and process design, and in some contexts also economics, supply chain management, chemicals/materials data management and integration with enabling digital technologies. Safe-by-design sits at the interface between chemicals, materials, products and services.
- ***Relevant actors*** need to be involved. Communication in supply chains is required – between end users (businesses or consumers), producers of mixtures or articles, chemical producers and/or producers of alternative materials, retailers and producers of secondary raw materials.

Note that the first three elements refer primarily to the content of safe design, while the other two are more process-oriented.

These elements need to be made operational following three funding areas for a Horizon Europe programme:

- <u>Developing or improving methodologies</u>: reliable and suitable methodologies for safe (re)design of chemicals and materials have to be (further) developed to ensure that toxicity and other lifecycle considerations (including circularity) are integrated into design processes.
- <u>Addressing thematic Research, Development and Innovation (RD&I) needs</u>: RD&I is needed to overcome technical and scientific challenges in areas where it has been difficult to find safer alternatives. Such RD&I should be based on a functional approach, which means that the focus is at the function performed by chemicals (e.g. water and dirt repellency, fire safety, preservation etc.) rather than the chemical structure as such. Methodologies for safe-by-design need to be applied to (re)design and assess solutions for different applications, avoiding the use of hazardous chemicals whilst improving by design the lifecycle safety and sustainability profile. This can be done at potentially very different levels (chemical, material, product, process, business models), including non-chemical solutions.[29] Thus far, most research has been conducted at chemical substances level (chemical-by-chemical substitution). Innovating on material structures, product and process improvements can be given more emphasis, as part of the functional substitution

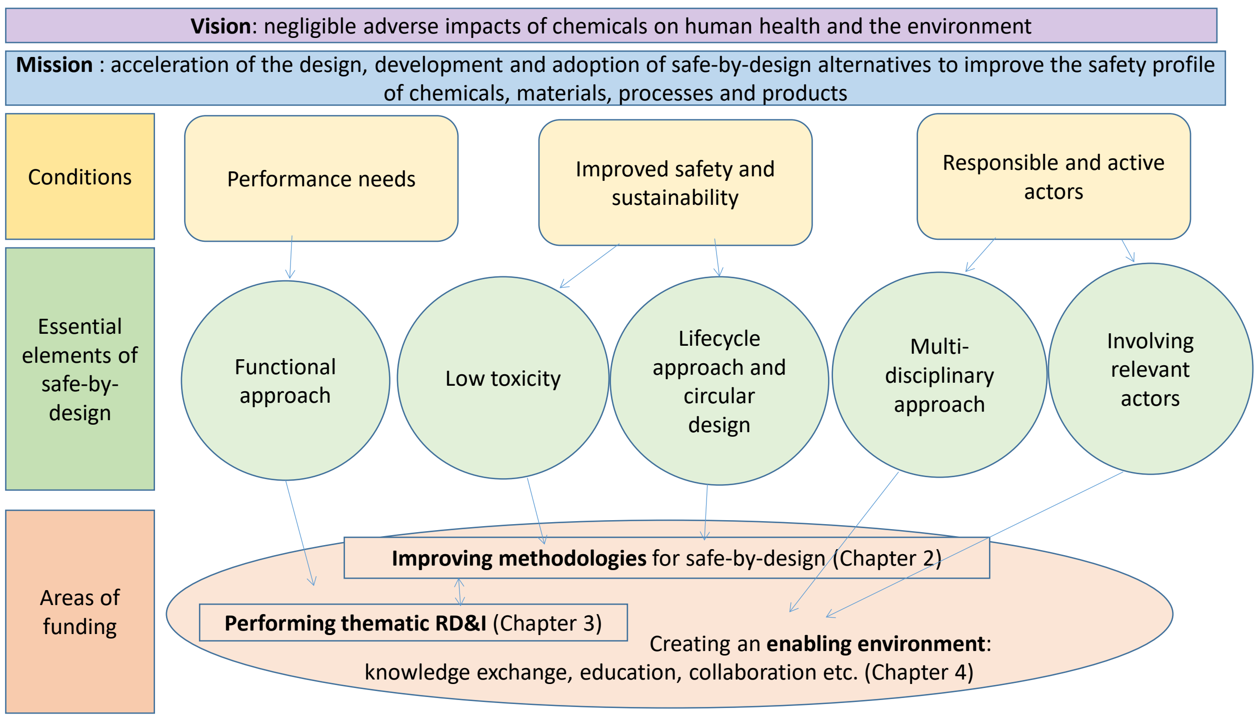
[29] the term 'non-chemical solutions' may not be fully accurate, since alternative materials or technologies will also involve chemicals. However, this term is meant to also refer to alternatives where the function previously performed by hazardous chemicals/additives could now be provided by innovation at the levels of materials, products, services or processes.

concept. This also means that assessments of toxicology and other sustainability aspects need to cover materials, products and processes as a whole. This broader perspective brings about the involvement of other disciplines and stakeholders across value chains and sectors.

- Creating an enabling environment: Safe-by-design - as a new interdisciplinary approach - needs to be set up, to develop terminology, methods and tools. Knowledge exchange, education/skills and supply chain cooperation are important aspects of an enabling environment. Awareness raising is paramount because safe-by-design involves a change in mind-set in businesses, including at the executive positions. Activities not primarily focused on research but aimed at networking, awareness raising and education can also be part of EU innovation programmes.

Subsequent chapters will discuss each of these aspects in more detail.

*Figure 1.1 Conditions, elements of safe-by-design and proposed areas of EU funding*



# 2 RESEARCH NEEDS FOR METHODOLOGICAL DEVELOPMENT

## 2.1 Introduction

This chapter provides an overview of research needs for methodological development for safe-by-design. These will address three essential elements mentioned in Chapter 1: the functional approach, minimising toxicity and the life cycle approach.

Safe-by-design builds on elements of existing assessment and management frameworks with their specific focus points, for which data, models, and extrapolation tools exist and are being continuously improved. Such frameworks include qualitative, semi-quantitative and quantitative approaches applied in chemical safety assessment, health impact assessment, product life cycle assessment, cost-benefit analysis, high-throughput risk screening and chemical prioritization, alternatives assessment and chemical substitution.[30] At a higher level, green chemistry and sustainable chemistry are approaches that aim to integrate various frameworks.[31] The different frameworks are usually tailored toward answering specific questions with various purposes (e.g. protection versus prioritization), scope (consumer exposure versus emission over entire life cycle) and context (voluntary versus regulatory). They therefore need to be combined and adapted.

The consultation process described in the introduction resulted in the following research needs, which will be discussed below:

- criteria and targets;
- efficient ‘preventative’ toxicology and life cycle tools;
- accessible data;
- standardisation.

Additionally, stakeholders highlighted the need to develop methodologies as such to address the new complexity: transitioning from linear to circular economy but also the overall weighting and assessment of the sustainability profile of any alternative solutions.

## 2.2 Criteria and targets

In line with the functional approach, design processes need to take a broader view of performance needs and possible types of solutions considering different levels (chemical, material, product, service etc.), including non-chemical solutions.[8] This is not primarily a methodological research need, but a matter of combining all relevant disciplines in the design process and the setting of relevant criteria and targets. Such a process could also involve a critical review of technical specifications (see Chapter 4).

Safe-by-design requires that certain criteria and targets are used early in the design process. For several applications, such as flame retardants and curing agents, stakeholders have pointed at the lack of standardized alternatives assessment frameworks.[32] Several reports[33] underline the need for more harmonized criteria for what is considered ‘safe’ (or broader: sustainable), also in view of the

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[30] See e.g. Fantke P., Ernstoff A. (2018) LCA of Chemicals and Chemical Products. In: Hauschild M., Rosenbaum R., Olsen S. (eds) Life Cycle Assessment. Springer, Cham (Figure 31.1) for a non-exhaustive contrast of different assessment frameworks.
[31] See e.g. K. Kümmerer, Angewandte Chemie International Edition, 2017; C. Blum et al. Sustainable Chemistry and Pharmacy 2017, Circular Chemistry Slootweg et al, Nature 2019.
[32] Wood and CSES (2018), Safe Chemicals Innovation Agenda.
[33] OECD (2019), Workshop on Approaches to Support Substitution and Alternatives Assessment; Wood and Lowell Center for Sustainable Production (in prep.), Innovation Action Agenda for the Transition to Safe Chemistries and Technologies.

current diversity of labels and assessment methods. Such an effort would essentially be a consensus-building activity rather than (only) research. Two points of attention can be mentioned here.

The first one is that methods are needed that build on comparative and qualitative and, where possible, quantitative metrics to ensure consistency in design evaluation and prioritization for (re)design. This makes it possible to measure progress towards targets. It also would avoid that various aspects (e.g. consumer exposure, worker exposure, environmental emissions, water pollution) are assessed separately using different data and models (following different regulations). It also requires harmonisation of methodologies across regulations.[34]
A second attention point is the need to be aware of value-laden aspects and scientific complexities of choosing targets and the base for comparison. Fantke and Illner (2019) argue that research is required to develop science-based targets in line with overarching societal goals for human and ecological health (such as the Sustainable Development Goals). Such targets not only apply to toxicological aspects, but also to impacts associated with climate change, radiation, acidification and eutrophication, and resources depletion including land, water, mineral and energy resources.[35] These targets should be based on respecting ecological capacities for handling inputs (e.g. chemical emission) and outputs (e.g. extraction of water and other resources) and based on well-founded thresholds and quantifiable metrics.[36] Fantke and Illner (2019) consider that an absolute perspective is required, linking design performance to such measurable health targets. Relative assessments (e.g. comparison with an original design or comparisons across available options) are in their view insufficient, since the nature of limits for human and ecological health is absolute, and increasing overall pressure (e.g. increase in human population count, per-capita material and product demand) is currently outweighing most relative improvements. It is also essential to consider that capacities vary across regions and in time and are interdependent.[37] It is not clear whether this approach is always possible given the scientific complexities (data needed, interdependencies) and whether consensus can be achieved given the value-laden choices, such as the choice of allocation principles or the level of evidence considered appropriate to identify a certain effect. One approach to address the subjective choices involved in the allocation of 'environmental space' at the level of e.g. products or companies could be to test and contrast several allocation methods (presumed that data are available).[38] Any attempt to reach consensus on harmonised safety criteria will probably need to have some common elements as well as flexibility to incorporate different viewpoints and contexts for comparison.

### 2.3 Efficient 'preventative' toxicology and life cycle tools

There is a need for validated and harmonised tools that assist the design process to find solutions with lower toxicity. Many methods exist for the assessment of existing alternatives to hazardous chemicals. However, fewer methods are available specific to *de novo* design that help designers to avoid substances and materials with undesirable properties. Such methods include qualitative structure-based or physicochemical property-based design filters for the first design stages, and more refined

[34] Amec Foster Wheeler, Trinomics and Technopolis (2017), Study to support the Fitness Check on the most relevant chemicals legislation.

[35] For an overview: Y. Dong and M.Z.Hauschild (2017), Indicators for Environmental Sustainability. Procedia CIRP Volume 61, 2017, Pages 697-702.

[36] See e.g. A. Bjørn, M. Margni, P. Roy, C. Bulle, M.Z. Hauschild (2015) A proposal to measure absolute environmental sustainability in life cycle assessment. Ecological Indicators 63 (2016) 1–13.

[37] P. Fantke and N. Illner (2019), Good that are good enough: Introducing an absolute sustainability perspective for managing chemicals in consumer products. Current Opinion in Green and Sustainable Chemistry 2019, 15:91–97. See also: M.Z. Hauschild (2015), Better – But is it Good Enough? On the Need to Consider Both Eco-efficiency and Eco-effectiveness to Gauge Industrial Sustainability. Procedia CIRP, Volume 29, 2015, Pages 1-7; A. Bjørn and M.Z. Hauschild (2012), Absolute versus Relative Environmental Sustainability. What can the Cradle-to-Cradle and Eco-efficiency Concepts Learn from Each Other? Journal of Industrial Ecology, Volume 17 nr 2. P. 321-332.

[38] M.W. Ryberg, M. Owsianiak, J. Clavreul, C. Mueller, S. Sim,H. King, M.Z. Hauschild (2018), How to bring absolute sustainability into decision-making: An industry case study using a Planetary Boundary-based methodology. Science of the Total Environment 634 (2018) 1406–1416.

tools for further assessment, such as *in silico* modeling of mechanisms and QSAR (Qualitative Structure - Activity Relationship) and QSDAR (Quantitative Spectroscopic Data Activity Relationships).[39] Experiences in the design of pharmaceuticals (e.g. for biodegradability) have been suggested to use more broadly in chemical design.[40] More generally, stakeholders have highlighted links of these types of tools with innovation in digital technologies.

Considering impacts along full chemical, material and product life cycle ranges is broadly accepted to play a key role for achieving environmental sustainability. While life cycle assessment data and methods are being continuously improved and advanced, the current methodological framework is far too complex to be useful in a safe-by-design context, which requires rather efficient and flexible methods based on, for example, high-throughput data and models. Such approaches should be further refined and extended to make it possible to check hundreds of thousands of chemical-product combinations relatively quickly. Streamlined approaches, hence, need to be developed and harmonized across impact categories and life cycle stages in terms of underlying assumptions, level of detail and uncertainties.

According to Coish et al. (2016), existing *in silico* approaches to toxicity prediction vary widely in accuracy for various end points due to the inherent complexity of toxicity pathways and limited availability of quality data sets. They, however, expect a significant future potential through computational chemistry coupled with high-throughput and mechanistic toxicology. Such an iterative process would allow the development of guidelines for a priori molecular design and will reduce reliance on predictive *in silico* assessments of chemical toxicity a posteriori ('preventative' rather than 'predictive' toxicology).[41] This suggests that in the absence of reference systems for *in silico* methods for new substances, rapid *in vitro screening* can be helpful, and in the long term helps to improve *in silico* modelling.

Whereas methods for alternatives assessment usually aim at the molecular level, assessment and comparison of alternative materials is an emerging field, which, given the multiplicity of chemicals and additives in a material, is quite challenging. On difficulty will be to take account of the multiparametric toxicity of a great number of chemicals in a material. In the preparation of this non-paper, stakeholders also highlighted the need to adapt existing LCA models to new materials.

In fact, the above directions point at the integration of hazard/risk assessments, LCA methodologies and circular design. LCA methodologies usually only cover hazard/risk assessments at a highly aggregated level.[42] It also underlines the need for designers within companies to have greater understanding of predictive toxicological methods, and for such methods to be aligned with their design workflow requirements.

### 2.4 Accessible data

A third area of methodological development is making data available to designers in an appropriate way. The FAIR data approach aims to make data Findable, Accessible, Interoperable and Reusable, and has implications for both data generation and data management, including for data about toxicological hazards. An important action in this context is to develop harmonized formats for FAIR data that can be used as requirements for research funding. In the context of the Horizon 2020 funded Gov4Nano project, such a harmonized format for nanomaterials is being developed. Meta-

[39] The National Academies (2014). A framework to guide selection of chemical alternatives.
[40] See Kümmerer Sustainable Chemistry and Pharmacy 2019.
[41] P. Coish, B.W. Brooks, E.P. Gallagher, T.J. Kavanagh, A. Voutchkova-Kostal, J.B. Zimmerman, P.T. Anastas (2016), Current Status and Future Challenges in Molecular Design for Reduced Hazard. ACS Sustainable Chemistry & Engineering 4:5900−5906.
[42] Ernsthoff et al. (2018), Challenges of including human exposure to chemicals in food packaging as a new exposure pathway in life cycle impact assessment. The International Journal of Life Cycle Assessment, Issue 3/2019.

information about data quality (e.g. whether data have been subject to independent review) is important in this context as well.

Stakeholders have highlighted the need for open access databases with hazard profiles of existing and emerging chemicals.[43]

A related area of work is the development of transparent, efficient, and reliable methods that allow for information transfer along chemical, material and product supply chains. Any confidentiality concerns will need to be addressed in such efforts. Existing methods, such as block chain approaches, constitute a valuable starting point, but are currently largely constrained by important challenges that vary across sectors (e.g. chemical versus electronics versus agrifood industry), regions (e.g. different regulatory conditions), and capacities (e.g. industrialized versus developing countries).

Including all of the above aspects about data accessibility in an innovation programme for safe-by-design would enlarge the scope too much, but some activities could be taken on board where they are important to increase adoption of safer alternatives. In any case, the interoperability of research efforts with data formats, standardization and quality of data, confidentiality, open access databases/data sharing platforms, and methods for information transfer and management needs to be ensured.

### 2.5 Standardisation

Being an aspect of all of the above methodologies, standardization can play an important role to ensure harmonization, trustworthiness and transfer of information along the supply chain. This applies to both assessment methods and data fed into them to assess safety and overall sustainability. The OECD brings together many standardised test methods to assess potential effects of chemicals on human health and the environment. In addition to methodologies mentioned in the above sections, relevant standards in the context of safe-by-design include:

- methods to measure concentrations of (new) chemicals used in materials and/or to assess toxicity of materials and products, to ensure possibilities for recycling;
- standards for product performance;
- related standards for circularity and/or separability of products;
- standards for data quality and tools.

In general, the European Commission encourages researchers to address the relevance of standards in their projects[44], since standardisation is a powerful tool to bring research and new technologies to the market. It can also significantly contribute to dissemination of research results. It is therefore recommended to involve standardisation bodies in safe-by-design RD&I projects to make full use of existing standards and also to establish new areas of standards activity.

### 2.6 Summary

We summarize the needs for methodological development in table 2.1. Promoting these priority research areas should involve evaluation, harmonization, consolidation and standardization, with a broad involvement of the scientific community, design practitioners, industry, policy makers, and international non- and inter-governmental organizations.

[43] Wood and CSES (2018), Safe Chemicals Innovation Agenda.

[44] Regulation (EU) No 1025/2012 of the European Parliament and of the Council of 25 October 2012 on European standardisation. See also ftp://ftp.cen.eu/PUB/Publications/Brochures/STAIR.pdf.

*Table 2.1 Overview of methodological RD&I needs for safe-by-design*

| | RD&I focus areas |
|---|---|
| **Criteria and targets** | • Harmonised and validated criteria and science-based targets for safety and sustainability for the whole life cycle of service/product/material/chemical, also enabling the transition to circular economy |
| **Efficient 'preventative' toxicology and life cycle tools** | • Methods and digital tools for integrating knowledge of toxicity into early design and to evaluate sustainability impacts throughout the lifecycle |
| **Accessible data** | • Make data available (criteria for Findable, Accessible, Interoperable and Reusable data in research calls, add data to open access databases) |
| **Standardisation** | • Involve standardisation bodies to ensure optimum use of standards and development of new standards (data, methods, tools) |

# 3 ADDRESSING THEMATIC RD&I CHALLENGES

## 3.1 Introduction

The methodologies discussed in the previous chapter should aim to be applied to new designs for any chemical application to avoid future hazards. They can thereby be applied to re-design chemicals, materials, products and services in certain thematic areas where safety and sustainability concerns arise and have proven hard to solve. This chapter aims to identify those thematic areas for research, development and innovation (RD&I).

We discuss research themes in three sections, related to functionalities of **materials**, **formulations** and **industrial processes** respectively, acknowledging that overlaps among these clusters exist. Within the themes, there are research directions at different levels: materials, products, processes and chemicals. It can be observed that thus far, most research has been conducted at chemical substances level (chemical-by-chemical substitution). Innovating on materials' structures, product and process improvements can be given more emphasis, as part of the functional substitution and safe-by-design concepts. This implies the involvement of multiple disciplines and stakeholders.

This chapter builds on the Safe Chemicals Innovation Agenda[45] and intends to cover the majority of functions provided by industrial chemicals. It is not exhaustive, since e.g. pharmaceuticals, pesticides, fertilisers, and heavy metals used for energy storage (batteries) are not elaborated. The working group supplemented the SCIA with additional insights based on its own expertise, additional consultations, and new publications. In addition, a workshop organised by SusChem (SusChem SIRA workshop, May 16-17 2019) was used to gain additional input from stakeholders.[40] Moreover, within the context of the latter, additional functionalities were suggested for further consideration:

- materials: UV-stabilisation and anti-oxidation for materials, in particular related to paints and coatings;
- formulations: stabilization (e.g. foams, emulsions, suspensions), colorants (dyes or pigments) and mechanical abrasives;
- process applications: preservation (e.g. process fluids), additives (e.g. softeners) and fuels.

A similar approach and methodologies may also apply for these functions.

Stakeholders also highlighted some cross-cutting aspects that are relevant under any RD&I theme. In particular, transitioning to circular economy and the emerging element of feedstock variability (waste or biomass, with potentially variable components) has been mentioned, especially at process, materials and product level. It is also recognized that safe-by-design is a multifunctional and highly complex challenge and innovations should account for the overall sustainability profile. Furthermore, scalability of the solutions is important to achieve maximum impact. Stakeholders have also highlighted the links with parallel innovation on waste treatment as well as separation and purification technologies.

## 3.2 Materials applications

In regards with safe-by-design of materials, stakeholders consulted generally emphasized the need for compatibility between safety and functionality, both in production and the final material and product. Feedstock variability mentioned above was seen as a potential source of additional safety considerations. Overall, there should be a drive for long-term alternatives rather than short-term and intermediate solutions. Horizontal actions also relevant to this functionality such as interdisciplinarity requirements in RD&I, LCA models adapted to new materials, materials design (modelling – enabling

[45] Wood and CSES (2018), Safe Chemicals Innovation Agenda.

implementation of digital technologies), and the respective education/skills development are further elaborated in Chapter 2 and Chapter 4.

#### 3.2.1 Repelling water, grease and dirt

*Context*

Water, grease and dirt repellence provides the resistance to the absorption or passage of water, oil or dirt resulting mainly from the application of surface treatment. Most currently applied treatments rely on per- and polyfluoroalkyl substances (PFAS). Overall, depending on the repellence effect obtained, currently, there are two types of materials: i) materials with inherent repellence properties (e.g. materials with compact, non-porous structures, being impermeable to liquid) and ii) materials with repellence finishing (e.g. coating or laminating technologies). PFAS are used for a wide range of industrial and consumer applications. Textiles (e.g. outdoor clothing), food preparation, and packaging are well-known areas, while other – less investigated - uses include cosmetics, inks, medical devices, pesticides, oil production and mining. PFAS are persistent in the environment and in some cases bio-accumulate in organisms.[46] Most research has focused on substituting long-chain PFAS. In recent years concerns have extended to (some of the) shorter-chain PFAS, for which less data are available. Among these concerns are the effects on drinking water supplies, in view of the mobility of the short-chain alternatives.[47] [48]

*RD&I challenges*

Focusing on meeting technical/materials performance, several alternatives have been reported, especially in regards with water-repellency.[49] Most discussed water-repellent alternatives are silicone-based agents (free from the persistent cyclic impurities); mixtures of silicones and stearamidomethyl pyridine chloride, sometimes together with carbamide and melamine resins; waxes and paraffins, usually modified melamine-based resins; structures, so-called dendrimers, which imitates the ability of the lotus blossom to repel water. On water repellence, there are also some new approach examples such as tightly woven fabrics (reverse osmosis membrane) in the application of textiles or the development of materials with inherent superhydrophobic properties.[50] Overall, performance of alternatives is not always seen as sufficient for all applications and more data are often required on safety performance.[51] Finding alternatives to achieve grease- and dirt-repellence, appears to be more challenging; hence this is a key research challenge to address. In all approaches, there are implications on performance, cost and changes to value chains to address.

*Emerging RD&I goals*

1. **New materials design approaches to achieve inherent repellence performance function**
   New approaches to achieve inherent dirt, grease, water repellence (e.g. reverse osmosis membranes for fabrics) could be further developed, in the absence of additives.

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[46] POP review Committee (2018), Further Assessment of Information on PFOA, its salts and PFOA-related compounds. Addendum to the risk management evaluation on PFOA, its salts and PFOA-related compounds. UNEP/POPS/POPRC.14/6/Add.2.
[47] UNEP (2019), Global Chemicals Outlook, p. 307-310.
[48] For experiences with finding PFAS-free alternatives see the Swedish POPFREE project: www.swerea.se/en/POPFREE and SUPFES project: www.supfes.eu.
[49] For a systematic overview in textile finish applications, see J. Williams (2017), Waterproof and Water Repellent Textiles and Clothing'.
[50] KEMI (2015), Occurrence and use of highly fluorinated substances and alternatives.
[51] I.T. Cousins et al. (2019), The concept of essential use for determining when uses of PFAS can be phased out. Environmental Science: Processes and Impacts 2019.

2. **Innovative repellent materials with safer additives**
   Materials structure design and performance studies could be carried out, using alternative chemicals with positive scores on environmental degradability and ability to mineralise.

Stakeholders have also suggested as a common innovation action the upscaling of applications with intermediate technology readiness levels (TRL 4-6), such as in textiles. In this context, the organization of supply chains and enabling recyclability of new materials are important aspects.

### *3.2.2 Fire safety*

*Context*

The functionality of fire safety is currently provided mainly by flame retardants and firefighting foams. Flame retardants (FRs) are applied on the surface of, or incorporated in, combustible materials to lower product ignitability, fire development rates and smoke production. Often needed to comply with product flammability standards, they are applicable to a wide range of products including electronics, textiles, furniture, aviation, e-mobility, $H_2$ storage, construction and insulation materials. A wide variety of flame-retardant chemical classes are available, including halogenated (brominated and chlorinated), phosphorous-based (organic and inorganic), nitrogen-based, mineral fillers, inorganic compounds and nanocomposites.[52] Many halogenated compounds are classified as being persistent, bio accumulative, and toxic (PBT) and are associated with carcinogenicity, neurotoxicity and endocrine disruption.[53] However, halogen-free alternative FRs may also pose similar hazards though, and similarly to other themes, more data are needed not only on technical but also safety performance for any alternative solution(s).

*RD&I challenges*

Each sector/application must often meet its own stringent performance criteria and fire-retardant specification tests. This poses a challenge on developing safer FRs alternatives due to the large variety of materials and applications where fire retardancy is required. FRs being of reactive nature, they pose additional challenges regarding separation from waste streams (lifecycle implications). In all approaches to alternatives, there are implications on performance, cost and changes to value chains to address. Overall, research has so far mainly focused on identifying alternatives for main applications. In some niches, more solutions are available than others. Often many data on technical performance and/or safety (health and environment) are lacking, making it difficult to avoid regrettable substitution.

For firefighting foam applications (implications on groundwater and soil contamination), alternatives to PFAS-based foams have already developed and are applied in different parts of the world.[54] Whether or not fluorine-free foams have equivalent performance is a matter of debate. The scientific body of

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[52] Morgan, A. B. and Worku, A.Z. (2015) Flame Retardants: Overview. Kirk-Othmer Encyclopedia of Chemical Technology.
[53] S.D. Shaw, A. Blum, R. Weber, K. Kannan, D. Rich, D. Lucas, C.P. Koshland, D. Dobraca, S. Hanson and L.S. Birnbaum (2010), Halogenated Flame Retardants: Do the Fire Safety Benefits Justify the Risks? Reviews on environmental health 25(4):261-305 · October 2010.
[54] POP review Committee (2018), Further Assessment of Information on PFOA, its salts and PFOA-related compounds. Addendum to the risk management evaluation on PFOA, its salts and PFOA-related compounds. UNEP/POPS/POPRC.14/6/Add.2.

the Stockholm Convention has concluded that fluorine-free foams are comparable to fluorine-based foams in meeting relevant certifications for almost all uses with some exceptions.[55]

*Emerging RD&I goals*

For applications where a flame-retardant function in materials is considered essential for society there are the following RD&I goals:

3. **Innovative materials with inherently flame-resistant function.** These could include, as an example, new safe bio-based materials structures. Stakeholders consulted estimated current status at TRL 1-4 and the goal to reach in 2030 could be to reach TRL 6-7.

4. **Intermediate and temporary solution: materials design to reduce additive exposure/leaching to the environment**
   Alternatives could include for example reactive flame retardants that will become part of the polymer material and will not leach into the environment. Current solutions already exist at high TRLs and experts consulted recommended to stimulate further market uptake, stressing that these are merely intermediate solutions.

### *3.2.3 Plasticizing*

*Context*

Plasticizing refers to the functionality offered by organic compounds added to polymers to facilitate processing by modifying physical properties such as flexibility, fluidity and toughness. In Europe, mainly orthophthalates are used in a variety of applications, with 85% applied on flexible PVC.[56] Overall applications include wires, films, sheets, flooring, wall covering, tubes and coatings in construction, the automobile industry, furniture and textiles with many downstream processing industries relying on the functional properties provided by plasticizers. Other important applications include food packaging, medical products and consumers products (e.g. toys). The widespread application increases risks of high exposure of certain hazardous plasticizers. Plasticizers can leach out of products over time and diffuse into the air, water, food, house dust, soil and organisms. Health effects, such as endocrine disruption and damaging fertility and unborn children, have been reported for a number of phthalates.[57] [58] Phthalates are frequently encountered in waste streams (plastics, textile and paper), giving lifecycle implications.[59] [60]

*RD&I challenges*

RD&I solutions have focused on phthalate alternatives, often also bringing other characteristics such being bio-derived and biodegradable compounds. Alternative plasticizers, currently known, include

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[55] POP review Committee (2018), Further Assessment of Information on PFOA, its salts and PFOA-related compounds. Addendum to the risk management evaluation on PFOA, its salts and PFOA-related compounds. UNEP/POPS/POPRC.14/6/Add.2.

[56] European Plasticizers (2018), Factsheet. https://www.plasticisers.org/wp-content/uploads/2018/10/EP_Factsheet_OCT2018_EN_FINAL-1.pdf

[57] The Lowell Center for Sustainable Production at the University of Massachusetts: Phthalates and Their Alternatives: Health and Environmental Concerns, January 2011.

[58] KEMI (2015) Phthalates which are toxic for reproduction and endocrine-disrupting – proposals for a phase-out in Sweden: Report from a government assignment 4/15.

[59] K. Pivnenko, M.K. Eriksen, J.A.Martín-Fernández, E.Eriksson and T.F.Astrup (2016), Recycling of plastic waste: Presence of phthalates in plastics from households and industry. Waste Management 54 · May 2016.

[60] P.N.H. Wassenaar et al. (2017), Substances of very high concern and the transition to a circular economy An initial inventory. RIVM Letter report 2017-0071.

citrates, sebacates, adipates and phosphates, amongst others.[61] Nonetheless, data gaps and concerns about health and environmental effects often persist for the proposed alternatives as well. Other approaches include researching on alternative flexible polymers, requiring fewer, no or less harmful additives, and even the consideration of alternatives to plastic materials for specific applications. On the approach of alternative flexible polymers, the production without any hazards must be proved. When considering the replacement of plastic materials for specific applications, there can be a challenge on the equivalence in functionality (mainly flexibility and durability).

*Emerging RD&I goals*

For applications where a plasticizing function in materials is considered essential for society and the transition to circular economy (*design-for-recyclability*) there are the following research needs:

1. **Materials with the same functionality (flexibility, durability) in the absence of hazardous chemical substances (in final product and production process)**
   This could require alternative polymers and/or materials. All sustainability aspects in the life cycle need to be accounted for. Stakeholders indicated current status for such alternatives at TRL 3-4.

2. **Novel material/chemical combinations with plasticizing functions.**
   This includes materials with plasticizing functions using alternative chemical groups. Molecular level studies are needed to improve understanding of toxicological effects, in both the final product and the processing required for production, and implications on performance, cost and changes to value chains. This has been indicated as low TRL (1-3) with a possible goal to achieve TRL 5-6. Stakeholders highlighted the application of materials modelling towards advancing this further.

## 3.3 Formulation applications

For formulation applications, we will focus on preservation and surfactants functions. However, stakeholders have suggested as additional themes: stabilization (e.g. foams, emulsions, suspensions), colorants (dyes or pigments) and mechanical abrasives. For stabilization (particles), improvements are required in both functionality and sustainability. As a first RD&I action it was proposed to better understand the mechanisms of de-stabilization, to address complex multi-scale and multi-parameter effects. For colorants, where food and textiles applications where highlighted; challenges include meeting physical stability and a full range technical performance. Furthermore, research into solid mixtures (e.g. tires), going beyond classic formulations, was suggested. The consideration of solutions for use of preservatives in process fluids (going beyond the formulation functionality) was also highly recommended. The need for knowledge sharing platforms and cross-sectorial collaboration was also stressed (see Chapter 4).

### *3.3.1 Preservation*

*Context*

Preservatives are chemical substances preventing the growth of microorganisms, helping on maintaining the quality of a final product, increasing its shelf life and biosafety profile. Currently natural or synthetic ingredients are used including parabens, biocides, formaldehyde-based, calcium propionate, sodium nitrate, sulfites and disodium sulfite. Preservatives are added to many consumer

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[61] The Lowell Center for Sustainable Production at the University of Massachusetts (2011), Phthalates and Their Alternatives: Health and Environmental Concerns.

products, medical applications, food/ food packaging, paints, household products, wood and pharmaceuticals. Concerns have been raised, for example, for some parabens in personal care products, due to potential endocrine effects.[62] Some biocides used as preservatives in canned food, shampoos and soaps, and textiles, are known as skin sensitizers,[63] and some biocides used as wood preservatives are considered to bring hazards as carcinogenic or toxic for reproduction.[64] As for the previous themes, here more data are required on alternatives and research beyond chemical-by-chemical substitution.

*RD&I challenges*

The performance of alternatives can vary under different physicochemical characteristics such as pH, often requiring more complex reformulation to create equivalent physical and overall performance. Overall, alternatives present the challenge of having an application/use-specific technical performance in addition to their safety profile. Moreover, there is a need to develop more specific and targeted solutions, matching the preservation needs (increased specificity for the target organisms).

*Emerging RD&I goals*

3. **Alternative preservation systems based on alternative mechanisms.** This includes preservation systems, mostly non-chemical, based on e.g. heat treatment, electrostatic spraying, nanotechnologies etc. Stakeholders have highlighted the potential of a combination of physical and chemical treatment for preservation functionalities.
4. **Mechanisms of antimicrobial activity with new chemical-material combinations (raw materials combinations & design approaches).** This involves approaches such as 'systems' for preservation with different combinations of raw materials (synergistic efficiency) or design approaches based on biomimicry and nature-inspired solutions.

### *3.3.2 Functions provided by surfactants*

*Context*

Surfactants are used towards lowering surface and interfacial tension. These functions are based on unique characteristics such as amphiphilicity and solubility in polar and non-polar environments, micelles formation and adsorption to phase boundaries. Derived properties include emulsifying and dispersing power, wetting, foaming, suspending, and stabilizing power. Surfactants are often classified by: 1) feedstock for synthesis (renewable, non-renewable), 2) degradability and environmental effects, 3) application and 4) chemical structure. They are used in industrial and household applications such as detergents, personal-care products, paints, pesticides and petroleum products. The Safe Chemicals Innovation Agenda has focused on <u>detergents</u> due to the volume of use. Not all surfactants are equally harmful. For example, cationic surfactants are more toxic than anionic surfactants when biodegrading in the environment.[65] However, several types of surfactants (cationic, anionic and nonionic) or their degradation products can be toxic for organisms or disturb their endocrine balance, even though the larger part of compounds is degraded during waste water treatment.[66] In the context of the Detergents Regulation, much progress has been made to improve

[62] http://ec.europa.eu/health/scientific_committees/consumer_safety/docs/sccs_o_041.pdf
[63] Hahn, S. et al. (2010). Consumer exposure to biocides - identification of relevant sources and evaluation of possible health effects. Environ Health 9:7. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2841155/
[64] Dr. Lisa Bushby (2012), Exposure to biocides: possible health effects. https://app.croneri.co.uk/feature-articles/exposure-biocides-possible-health-effects?product=3
[65] M.J. Scott, M.N. Jones (2000), The biodegradation of surfactants in the environment, Biochimica et Biophysica Acta (BBA) – Biomembranes Volume 1508, Issues 1–2, 23 November 2000, Pages 235-251.
[66] E. Olkowska, M. Ruman, and Z. Polkowska (2014), Occurrence of Surface Active Agents in the Environment. Journal of Analytical Methods in Chemistry. Volume 2014. Article ID 769708.

biodegradability of surfactants in detergents and to reduce phosphorus content.[67] Quaternary ammonium compounds (QACs) are antimicrobial agents commonly found in cleaning solutions used in residential, commercial and medical settings. Some QACs are shown to reduce fertility in mice, the effects on human health being unclear.[68]

*RD&I challenges*

Challenges include the development of surfactants from existing feedstock/resources and alternative feedstock but innovate on biodegradability, according to standards, and the implementation of lifecycle assessment, with strong safety considerations. It has been stressed that adding alternative components has important knock-on effects on other chemicals in the mix, so the formulation as a whole often needs to be redesigned. There are also production /scale-up challenges involved in the production process of alternative formulations.

*Emerging RD&I goals*

5. **Sustainable production of alternative surfactants that combine safety and life-cycle sustainability performance**
   Several renewable feedstock-based alternatives are possible such as those based on coconut-oil, palm-oil or algae in addition to fossil feedstock. However, availability, overall sustainability (carbon footprint and impact on the local environment), safety and costs should be holistically evaluated for all alternatives.

6. **Formulation redesign with alternative surfactants whilst understanding complex behavior of new molecules in mixtures/formulations and implications of production scaling up**
   Innovation is needed for formulations with alternative surfactants that meet physical stability and performance criteria. This requires understanding the effect of alternatives in the presence of other co-formulation components. In addition, process models and computational systems have been suggested to model implications of scale up of the production process.

## 3.4 Process applications

For applications that are mainly related to processes, we will focus on solvents, process regulators and surface protection. Stakeholders mentioned, however, some additional functions. Preservation was discussed in section 3.3.1 in the context of formulations, but can also be a process functionality (e.g. process fluids), with possible exposure at a process level rather than resulting from products. Furthermore, additives (e.g. softeners) are also used to improve process performance. Fuels was mentioned as a third function. On biofuels, safety hazards where seen (during processing, application, storage and transport) related to variability in composition, as well as performance challenges (equipment corrosion) requiring further research.
As a general comment, a holistic view of all sustainability factors was stressed, including prevention of process-related accidents (full HS&E perspective) as well as material and energy efficiency. Economic actors (process CAPEX, OPEX) to allow implementation (scale-up) and therefore magnification of the impact was also emphasized. Horizontal actions were suggested to account for the potentially disruptive innovations at the process level, which may require adaptation of skills, machinery and waste management. Multi-stakeholders' involvement and knowledge transfer (see Chapter 4) was

[67] RPA/Mayer Brown (2014), Support to the Evaluation of Regulation (EC) No 648/2004 (Detergents Regulation).
[68] V.E. Melin, T.E. Melin, B.J. Dessify, C.T. Nguyen, C.S. Shea and T.C. Hrubec (2016), Quaternary ammonium disinfectants cause subfertility in mice by targeting both male and female reproductive processes. Reproductive Toxicology 59 (2016) 159–166.

stressed, as well as the need for LCA methodologies to prove the holistic benefits of new solutions (Chapter 2).

### *3.4.1 Solvents*

*Context*

Solvents have many applications with performance being driven by several properties such as polarity, viscosity and evaporation rates. Exposure toxicity but also other environmental hazards have been of concern for some types of solvents. Important subgroups are the polar aprotic solvents and chlorinated solvents that will be phased out because neurotoxicity and/or carcinogenicity.[69]

Many solvents are applied as degreasing agents (e.g. cleaning of textiles and metal surfaces), additives, to enable efficient application (e.g. paints, glues), stripping agents (e.g. paint, varnish, glue removers) but also extraction solvents, separation and reaction media – with relevance to the chemical and pharmaceutical industry, but also often critical for recycling processes.

Solvents is one of the most comprehensively regulated functional category of chemicals. This has driven innovation in various applications, such as water-based paints, and powder coatings, both in order to reduce VOC emissions, and the development of safer solvents in manufacturing industries (pharmaceuticals). The functionality of solvents is expected to play a major role in realizing the circular economy, for instance for washing and separating material streams such as textiles.

*RD&I challenges*

There has been an emerging class of bio-based solvents, with some being drop-in analogues () and others providing new and beneficial properties; albeit their safety profile advantages are not always guaranteed.[70] Ionic liquids have also been widely researched as alternative solvents, mainly addressing the volatility/exposure toxicity aspects and with many application areas being suggested. The pharmaceutical industry has even proceeded with developing safe solvent guides for selection across different synthetic and processing routes.[71] Main challenges for bio-based solvents often focus on cost and availability, resulting into finding those in niche applications. For many alternatives, more detailed data are needed in respect with the environmental and health hazards (accounting for the full lifecycle). Low VOC and zero VOC products are also available but may still emit semi-volatile organic compounds and/or face challenges in terms of performance or recycling efficiency. Overall, new solvents can also imply complex reformulation and changes to production processes on many industry sectors. Specific RD&I is needed for the various applications and processes. In general, overall sustainability over the lifecycle is an important consideration. A distinction can be made between innovation focusing on alternative solvents in products (e.g. coatings and paints) and solutions for alternatives to hazardous solvents (e.g. aprotic solvents) used in production processes. For the latter, there is a fundamental distinction between the search for alternative solvents and more fundamental process innovations. For example, in Massachusetts ultrasonic techniques in water have successfully been used to degrease and clean, possibly making the use of solvents redundant for key applications, such as metal degreasing.[72]

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[69] D. van Es (2017), Study into alternative (biobased) polar aprotic solvents, Wageningen University and Research. UNEP (2019), Global Chemicals Outlook (2019), p. 448.
[70] See also: RIVM (2018), Toxicity screening of potential bio-based Polar Aprotic Solvents (PAS).
[71] D. Prat, A. Wells, J. Hayler, Sneddon, C. R. McElroy, S. Abou-Shehada and P. J. Dunn, CHEM21 selection guide of classical- and less classical-solvents, *Green Chem.*, 2016, **18**, 288–296.
[72] www.turi.org/TURI_Publications/TURI_Chemical_Fact_Sheets/Trichloroethylene_TCE_Fact_Sheet/TCE_Facts/Alternatives.

*Emerging RD&I goals*

**11. Innovative materials with reduced surface treatment requirements**
This includes the development of materials (e.g. building applications) that do not require additional surface treatment with a paint or a coating and mainly upon their application on the material surface. Challenges in this area include not only allowing similar performance/robustness but also equivalent processing flexibly. Alternatively, solutions could apply to alternative paints and coatings of equivalent performance (e.g. in terms of fast drying and durability). Any surface modifications should still allow for ease of circularity/recycling (e.g. ease of coating removal upon recycling).
Stakeholders proposed some examples of technologies, as alternatives to solvents-based surface treatment that could be brought to pilot level. This included materials design solutions with the examples of biomimicry and stimuli-responsive materials (low TRL), plasma treatment (TRL 3-5) and electrostatic treatment (TRL 3-5) with the two latter referring rather to process innovation options.

**12. Process innovations to avoid hazardous solvents in production processes**
This could e.g. require process intensification within manufacturing, other separation steps in downstream processing, or novel processes (e.g. supercritical fluids-based processes).
Stakeholders have mentioned as examples: gas phase processes (instead of dispersion/solution-based processes), solvent-less processes, water-based processes, and new reaction routes that could allow the use of safer solvents and modular processes. Regarding the latter, the possibility to re-apply learnings from the pharmaceutical sector was mentioned. Overall, such process innovations were seen as disruptive innovations with high CAPEX costs and additional process risks to be addressed.

**13. Alternative formulations/chemicals for process solvents**
Promising alternatives, including bio-based alternatives, to solvents (such as aprotic solvents and toluene) have been identified or at first stages of development and need further development. More research is needed to fully understand the safety and sustainability profile of some alternatives, acknowledging that alternatives are not necessarily safer, and safe-by-design and overall sustainability assessment principles should be applied.

### *3.4.2 Process regulation*

*Context*

This section refers to chemicals that are used to influence the course of a reaction. Key process regulators are cross-linking agents and curing agents, used in polymerization processes to meet diverse requirements such as strength, toughness, durability of products, high gloss and high depth of color, UV protection, or resistance to abrasion. Both aromatic and aliphatic compounds are used in such processes.

Chemical curing agents to produce epoxy resins and polyurethane foams were highlighted as being of concern, as well as peroxide-based catalysts but with limited information on the latter.[73] Regarding epoxy resins, the curing process provides mechanical strength, chemical resistance and electrical insulation for applications ranging from paints to civil engineering. Aromatic amines and dihydrazide compounds are used for this process. Aromatic compounds have been identified as sensitizers and carcinogenic, and dihydrazide compounds are known to have diverse sensitizing effects.[74]

[73] Wood/CSES (2018), Safe Chemicals Innovation Agenda, p. 44.
[74] ECHA C&L Inventory information, https://echa.europa.eu/substance-information/-/substanceinfo/100.018.569

Polyurethanes are found in a variety of sectors such as insulation, coatings, adhesives, sealants, elastomers, and construction materials. Diisocyanates that are used in the production polyurethanes, are recognized skin and respiratory sensitisers.[75] [76]

*RD&I challenges*

During the preparation of the Safe Chemicals Innovation Agenda[77], stakeholders indicated that no viable alternatives have been found for the hazardous chemicals used as curing agents in the production of foams and resins. At the same time, cured polymeric materials often provide critical functions such as longevity and protection. The implied challenge therefore is to develop resins and foams that do not require curing agents. Safe-by-design solutions therefore need to focus at higher levels (material, process) rather than chemical replacement, possibly starting in niche markets. Complementary to safe-by-design solutions, incremental improvements (process and reaction design optimization) in current processes have been suggested to reduce environmental release and human exposure.

*Emerging RD&I goals*

> **14. Innovative foams and resins.** This could include new materials such as inherently strong and versatile polymers for industrial and commercial purposes that do not require curing agents. Research will be needed to test and ensure both the health/environmental safety and the technical characteristics. According to stakeholders consulted, solutions at high TRL levels already exist (e.g. switching from thermosets to thermoplasts, self-curing resins) and one of the main challenge remainthe cost and hence the scalability.

### *3.4.3 Surface protection*

*Context*

This is a theme with a broad range of subtopics that could include the surface treatment of plastics and metals. The surface treatment of metals and plastics is found in many types of industry including automotive, construction, industrial equipment, food containers, and electronics industry. Treatment provides properties such as durability, corrosion protection, anti-fouling and conductivity. Risks of occupational exposure and environmental risks are linked with metal surface treatment processes that involve substance such as chromium, cobalt, nickel or cadmium.

*RD&I challenges*

Currently, alternative solutions can take the following forms: i) a different approach to surface treatment systems. For example, electrolytic or chemical treatments competing with surface treatments by solvent-painting, ii) redesign the products or components from alternative materials, reducing the need for surface treatment or iii) a combination of the above combining alternative materials and different ways of treatment (e.g. vapor deposition of a metal, instead of copper/nickel/chrome plating).[78]

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[75] ECHA C&L Inventory information, https://echa.europa.eu/substance-information/-/substanceinfo/100.002.697
[76] Lockey, J.E. (2015) Isocyanates and human health: Multi-stakeholder information needs and research priorities, J Occup Environ Med; 57(1): 44–51. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4286799/
[77] Wood/CSES (2018), Safe Chemicals Innovation Agenda. P. 46.
[78] See also B. Navinšek, P.Panjan and I.Milošev (1999), PVD coatings as an environmentally clean alternative to electroplating and electroless processes. Surface and Coatings Technology. Volumes 116–119, September 1999, Pages 476-487.

*Emerging RD&I goals*

**15. Alternative materials that are inherently resistant to corrosion or fouling** as an alternative to surface treatment (e.g. polymers engineering, nanotopography, nature-inspired treatments such as using amphyphilic proteins or polypeptides.

**16. Development of new techniques for surface treatment.** New approaches could be based on fundamentally different technologies. For example, in the case of anti-fouling on ships, available and emerging techniques include ultrasonic sound, nanomaterials, wraps, silicones and UV.

## 3.5 Summary

Table 3.1 summarises the RD&I priorities identified in this chapter.

*Table 3.1 Thematic RD&I focus areas*

| **Theme** | **RD&I focus areas** |
|---|---|
| | *Materials* |
| **Repelling water, grease and dirt** | • New materials design approaches to achieve inherent repellence performance function (e.g. reverse osmosis membranes for fabrics)<br>• Innovative repellent materials using alternative chemicals with positive scores on safety and ability to mineralise |
| **Fire safety** | • Innovative materials with inherently flame-resistant function<br>• Materials design to reduce additive exposure/leaching to the environment (intermediate solution) |
| **Plasticizing** | • Innovative materials with the same functionality (flexibility, durability) in the absence of hazardous additives (in final product and production process)<br>• Novel and sustainable material/chemical combinations with plasticizing function |
| | *Formulations* |
| **Preservation** | • Preservation systems based on alternative mechanisms (e.g. heat treatment, electrostatic spraying, physical and chemical treatment combinations etc.)<br>• Mechanisms of antimicrobial activity with new chemical-material combinations (raw materials combinations & design approaches)<br>• Sustainable production of alternative raw materials that combine safety and life-cycle sustainability performance |
| **Functions provided by surfactants** | • Formulation redesign with alternative surfactants whilst understanding complex behavior of new molecules in mixtures/formulations and implications of production scaling up |
| | *Processes* |
| **Functions provided by solvents** | • Innovative materials with reduced surface treatment requirements<br>• Process innovations to avoid hazardous solvents in production processes<br>• Alternative formulations/chemicals for process solvents |
| **Process regulation** | • Innovative foams and resins |
| **Surface protection** | • Alternative materials that are inherently resistant to corrosion or fouling<br>• Development of new techniques for surface treatment |

Additional themes to consider are in the areas of pharmaceuticals, pesticides, fertilisers, heavy metals used for energy storage. In the preparation of this non-paper, stakeholders suggested as additional functionalities:

- materials: UV-stabilisation and anti-oxidation for materials, in particular related to paints and coatings;
- formulations: stabilization (e.g. foams, emulsions, suspensions), colorants (dyes or pigments) and mechanical abrasives;
- process applications: preservation (e.g. process fluids), additives (e.g. softeners) and fuels.

# 4 CREATING AN ENABLING ENVIRONMENT

## 4.1 Introduction

Technical research and innovation is not sufficient for safe-by-design inventions to get adopted. This chapter will discuss how the proposed RD&I can be embedded in a wider strategy that gives focus to the RD&I efforts itself and also involves additional policy interventions to encourage market introduction. We limit the discussion to those interventions that could be part of a programme within Horizon Europe.

## 4.2 The context of safe-by-design innovations

An invention has a much better chance of being adopted if during its development into a marketable substance, material, product or service the conditions of the specific context are being met. To some degree, those conditions can be actively altered if these pose barriers for desirable change. Such conditions differ between specific supply chains, which each have different market structures, cultures and patterns of competition or cooperation. The mix of actions needed therefore also differs between supply chains and also depends on technology readiness levels of emerging or existing innovations (emphasis on invention or on adoption).

Reports[79] have identified the following barriers to the uptake of safer alternatives:

- incumbency (difficulty for new entrants to compete with established low-cost and well-performing chemistries);
- lack of predictable and clear demand signals in global supply chains;
- different interpretations of 'safe' and 'sustainable';
- concern about 'risks of switching' (process changes, material incompatibility etc.);
- insufficient connection between regulatory priorities and RD&I activity;
- limited technical capacity for SMEs to evaluate or adopt substitutes;
- lack of transparency in the supply chain;
- limited knowledge and data sharing within and across sectors.

We will highlight two potential areas of funding in the next sections:

- knowledge development, networks and education.
- supply chain cooperation and need for coordination.

## 4.3 Knowledge development, networks and education

Safe-by-design requires a new interdisciplinary approach, involving chemistry, toxicology, sustainability assessment, industrial design, circular design, material sciences, digital technology, process technology and data management. In addition, a community of practice needs to develop, that will help to test the new paradigms, concepts and methods in practice. In the preparation of this non-paper, stakeholders highlighted the need for knowledge sharing platforms and cross-sectorial collaboration to identify and further develop research questions and share best practices.

Tickner and Jacobs (2016) conclude that there is a discrepancy between industry's needs to identify alternatives to hazardous substances (SVHCs, substances of very high concern) and the research base in academia and other research institutes capable of identifying sustainable chemical or non-chemical

[79] http://www.greenchemistryandcommerce.org/documents/Advancing-Green-Chemistry-Report-June2015.pdf, and Tickner and Jacobs (2016). Improving the Identification, Evaluation, Adoption and Development of Safer Alternatives: Needs and Opportunities to Enhance Substitution Efforts within the Context of REACH. See also UNEP (2019), Global Chemicals Outlook, p. 68, and for the textile sector: KEMI (2014), Chemicals in Textiles. Risks to human health and the environment. P. 74.

alternatives for these substances.[80] According to OECD (2019), there is a need to create support for knowledge sharing, data sharing, sharing of information on existing and emerging alternatives and sharing of business opportunities'.[81] Therefore, Wood and Lowell (in prep.) recommend to establish an EU-network Safer Chemistries and Technologies Innovation Support Network.[82] This may also help to overcome some of the barriers mentioned above, such as the different interpretations of 'safe' and 'sustainable' and the limited technical capacity for SMEs to evaluate or adopt substitutes. Some countries (e.g. Sweden and Denmark) have set up support centres to facilitate such networking at national level.

Research programs and calls may stimulate the building of networks and communities of practice as an objective (e.g. Coordination and Support Actions) or by involving these as a necessary condition in thematic projects. An example in the context of nanotechnology research is the RATA project of the Dutch program Nanonext.nl. In this project, students and academics can participate, and give and receiving trainings as part of their research projects. Other examples are the KICs (Knowledge and Innovation Communities) within the EIT (European Institute of Innovation & Technology), which focus on technology scale up, implementation and education. Some current KICs (raw materials and manufacturing) have connections with safe-by-design and have developed educational products targeted at students, doctoral students, industry professionals and the wider public.

At a more fundamental level, a mindset is needed in which scientists in academia and companies are aware and appropriately trained to contribute to safer innovations and responsibilities along the supply chain. From the very start of academic education, safety aspects should be included in learning goals, in curricula, bootcamps and extracurricular activities and in-company training. Currently, students in chemistry receive little education about toxicology, while toxicologists are rarely involved in design processes, and if so, only at the later stages. Interdisciplinary education is therefore needed where chemists/engineers are trained alongside toxicologists and health/environmental scientists.

Usually learning goals and curricula are set at institutional or national level, so this is a bottom up process and not easy to influence at EU level. This process can, however, be stimulated and facilitated by extracurricular facilities like international summer schools and workshops, challenges and competitions, internships, fellowships, international educational networks, also including post-doc research. This could also extend to other fields such as industrial design, circular design, material sciences, process technology and data management.[83] An example of this approach is the master programme for sustainable chemistry at Leuphana University which starts in 2020.[84] Large companies can also play an important role for some types of training, such as challenges to enable startups to further develop their innovations (e.g. Imagine Chemistry from Nouryon or CEFIC bootcamps[85]).

The implementation of digital technologies to enable the design and assessment of safer chemicals, materials and processes along their lifecycle and the necessary education and skills should also be fostered.

A landscape analysis could make more clear what disciplines can contribute in which ways, which existing networks can be built upon, and which research and education institutes can contribute.

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[80] Tickner and Jacobs (2016). Improving the Identification, Evaluation, Adoption and Development of Safer Alternatives: Needs and Opportunities to Enhance Substitution Efforts within the Context of REACH.
[81] OECD (2019), Workshop on Approaches to Support Substitution and Alternatives Assessment.
[82] Wood and Lowell Center for Sustainable Production (in prep.), Innovation Action Agenda for the Transition to Safe Chemistries and Technologies.
[83] See also UNEP (2019), Global Chemicals Outlook. P. 61-65.
[84] https://www.leuphana.de/en/professional-school/masters-studies/sustainable-chemistry.html
[85] https://cefic.org/media-corner/newsroom/shining-a-light-on-green-chemistry/.

## 4.4 Supply chain communication and need for coordination

User-driven cooperative innovation does not happen when applying traditional innovation paradigms, where a producer innovates to reach its own goals. Such innovation depends on management that oversees the entire innovation effort and the contributions of all stakeholders. When too many different stakeholders are necessary to develop, test, perfect and adopt an innovation, there is a large risk that no individual stakeholder has a sufficiently large interest and has sufficient knowledge and capabilities to drive it forward. This also holds for many safe-by-design challenges. Furthermore, innovation is not a one-way street, but an iterative process, in which experiences and (scientific) questions along the line should lead to adaptations of the design. For these reasons, dialogue and collaboration in supply chains, organized by a neutral facilitator, is needed. Some of the barriers mentioned above can be addressed in such collaborations (although not entirely solved), such as lack of transparency in the supply chain and concerns about the risks of switching. The global and complex nature of supply chains also puts certain limits on possibilities to bring all actors together.
It is crucial in such processes to gain a detailed understanding of user needs and requirements to direct the innovation process. This could include downstream user companies, consumers, recyclers, investors and organizations involved in standardization. Technical specifications can in some cases also be reviewed or differentiated between different applications (for example repellency standards could be more strict for protective gear than for leisure jackets). This also addresses the problem that often hazardous chemicals need to be substituted by a combination of different alternatives to match the technical specification (in greater amounts to reach the same function).

We recommend to include a scoping stage with stakeholders in any thematic RD&I project before performing actual technical research. The purpose of this scoping stage would be to thoroughly analyse the situation/status-quo (e.g. chemicals currently used) and the context, to make the goals more concrete, and to align on the direction to the levels for finding solutions (chemical, material, process, product, service). Linked to the definition of objectives is the discussion about essential versus non-essential uses; Cousins et al. developed an approach to structure such discussions.[86] Other aspects to address in the scoping stage could be an analysis of the technical readiness levels (TRLs) of the alternatives, setting science-based criteria and targets, early-stage safety and LCA assessment, but also readiness of consumers and business models. Existing models for supply chain dialogues are the workshops within ECHA's substitution strategy, which often follow a specific format[87] and projects of the Green Chemistry and Commerce Council in the USA.

An innovation process as envisaged above is difficult to organize just by the individual actors, and should also not be invented anew for each invention, product, supply chain. A coordinating body or organization, preferably within a EU research program, could streamline and support those processes.

There are also other functions that could be performed by a central body, organization, network or platform. A central independent point could collect and evaluate best practices and information and make this accessible. Wood and Lowell (in prep.) recommend to better disclose information about chemicals used, their hazards and available alternatives. One action could be to develop harmonized positive criteria for safer chemicals and create an inventory of such chemicals. Experiences in the USA (Safer Choice) and in the textile sector (Blue sign system, textile industry dialogue in Sweden) can be built upon.

[86] I.T. Cousins et al. (2019), The concept of essential use for determining when uses of PFAS can be phased out. Environmental Science: Processes and Impacts 2019.
[87] https://echa.europa.eu/nl/substitution-supply-chain-workshops.

### 4.5 Summary

Additional interventions are needed to supplement research on methodological and thematic issues. Such interventions help to shape research activities themselves and also to address some of the barriers in the wider context. The mix of actions needed differs between supply chains and also depends on technology readiness levels of emerging or existing innovations.

A new research (inter)discipline and/or community of practice needs to develop, with scientists and innovators that develop in a coherent way necessary paradigms, concepts, methods and tools. These changes should involve all actors and stakeholders, such as scientists, innovators, laboratory employees, producers, downstream users, consumers, producers of secondary raw materials and regulators. This is a complex task needing a solid infrastructure. Table 4.1 summarises some possible activities that could fit within a programme.

*Table 4.1 Possible interventions to create an enabling environment*

| **Type of intervention** | **RD&I focus areas** |
|---|---|
| Knowledge development, networks and education | • Network building as objective or condition in funded projects<br>• Extracurricular activities, challenges and competitions, bootcamps, educational networks as start of a process of internalizing safe-by-design in education and skills development<br>• Landscape analysis of existing disciplines, networks and organisations |
| Supply chain cooperation and need for coordination | • Scoping phase with stakeholders before technical research to:<br>1) analyse context of the innovation (potential barriers)<br>2) identify user needs and performance criteria<br>3) identify appropriate levels of research (material, process, product, chemical)<br>• Coordinating body with research programme to oversee learning and innovation processes, and to make information available<br>• Data and knowledge sharing platforms across value chains and different sectors |

# ANNEX 1 EXPERTS CONSULTED FOR PREPARATION OF THE NON-PAPER

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