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Opportunities and obstacles for a green chemical industry in Sweden

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MISTRA SAFECHEM

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Contents

Abstract

This report summarises the results of a set of initiatives taken to identify opportunities and obstacles for the vision to enable a safe, green and sustainable chemical industry, and ultimately reduce the exposure of humans and ecosystems to hazardous chemicals. It represents a mid-term result in the Swedish research programme Mistra SafeChem's work to present vision and agenda for green chemistry in Sweden. The target group for this report is internal (Mistra SafeChem programme partners) as well as external for all parties interested in the transition to a safe, green and sustainable chemistry.

The report is based on the results of several activities/components: an overview of existing concepts for "Green Chemistry", industry initiatives and the EU Chemical Strategy for Sustainability; a previously published mapping of the Swedish chemical industry; a compilation and analysis of data on import, production and use of selected chemical groups from the Swedish products register and the results of interviews with representatives of chemical industries in Sweden are summarised.

Based on the results of these activities a number of obstacles and opportunities have been formulated along with general conclusions and recommendations for the enabling of the transition to a safe, green and sustainable chemistry. The main conclusions can be summarised as:

- The EU Chemical strategy for sustainability and associated industry initiatives as well as current and planned research initiatives provide a strong framework for coordinated action towards a vision of safe, sustainable and green chemistry.

- Chemical value chains are complex, international/global and include all societal sectors. Mapping chemical production and use with the purpose of analysing risks and prioritising areas for action/development is thus difficult and involves many actors. The chemical industry is also a heterogenous group of companies with activities ranging from small scale production of *e.g.* speciality chemicals and pharmaceuticals to large-scale production of base chemicals for a variety of applications and value chains. Different parts of the chemical industry also have widely differing conditions in terms of markets and market competition, industrial infrastructure, financial strength which all affect the possibility for change and introduction of new green and sustainable production methods and products.

- Research, innovation and investments are central to the future development. Specific challenges are the needs for reliable and low-cost tools for assessment of chemical hazards of both new chemicals and existing chemicals in new materials and applications, and for assessing hazards and risks of chemicals and materials in a life cycle perspective. This is also important in relation to the development of methods to operationalize the Safe and Sustainable by Design concept. Other challenges are the development of innovative production processes, chemicals and materials which fulfil criteria of safety and sustainability and contribute to societal needs including abatement of climate change.

Towards a vision and agenda for a Safe, Green and Sustainable Chemistry

Mistra SafeChem is a four-year research programme with six research partners and 14 industries represented. The overarching vision is to enable and promote the expansion of a safe, green and sustainable chemical industry. The vision covers all parts of the value chain from design/production to use and disposal of chemicals and materials. The main research components are to:

- Develop, test and evaluate innovative industrial production processes for non-hazardous molecules involving enzyme catalysis, and minimal waste processes.
- Develop and apply a robust framework for early prediction and verification of hazardous properties of new molecules or materials using *in silico* predictive models, *in vitro* tools and advanced chemical/biological analytical methods.
- Develop and apply improved methods for life cycle assessment incorporating hazardous properties of molecules and materials and risks for exposure along the full value chain.
- Conduct a series of case studies where specific design, production and recycling processes, in different levels of the value chain and representing a range of applications, will be evaluated.
- Develop a vision and agenda for expansion and implementation of the Mistra SafeChem concepts into Swedish chemical industry.

This report summarises the results of a set of initiatives taken to identify opportunities and obstacles for the vision to enable a safe, green and sustainable chemical industry, and ultimately reduce the exposure for humans and ecosystems to hazardous chemicals. It represents a mid-term result in the work aiming to present a final vision and agenda for green chemistry in Sweden. The target group for this report is internal (programme partners) as well as external for all parties interested in the transition to a safe, green and sustainable chemistry.

During the initial phase of the Mistra SafeChem programme, the EU Commission launched the Chemical Strategy for Sustainability (CSS) with a comprehensive set of initiatives to strengthen the protection of human health and ecosystems from chemical risks. The strategy also aims to ensure the contribution of the EU chemicals and materials industry to the transformation into a green, climate neutral and sustainable society. The research performed in the Mistra SafeChem programme can to a large extent directly contribute to the objectives in the Chemical Strategy. This political initiative has also provided a new framework of initiatives and future regulatory changes that is relevant to the programme.

In the first part of this report the definition of a safe, green and sustainable chemistry is briefly presented and discussed both from the perspective of the Mistra SafeChem programme and from the perspective of the EU Chemical Strategy for Sustainability as well as industrial initiatives from the European organisation SusChem. In the second part, results from a previously published mapping of the characteristics of the chemical industry in Sweden are summarized along with results from a compilation and analysis of data on import, production and use of selected chemical groups from the Swedish products register. In addition, the results of interviews with representatives of chemical industries in Sweden are summarised. Finally, some draft conclusions on the current opportunities and obstacles to enable a safe, green and sustainable chemistry are presented.

The report is thus a summary of several different internal and external activities in Mistra SafeChem, described in a flowchart in Figure 1. This flowchart also includes the link to the next and final step – to define a vision and agenda for a safe, green and sustainable chemistry in Sweden.

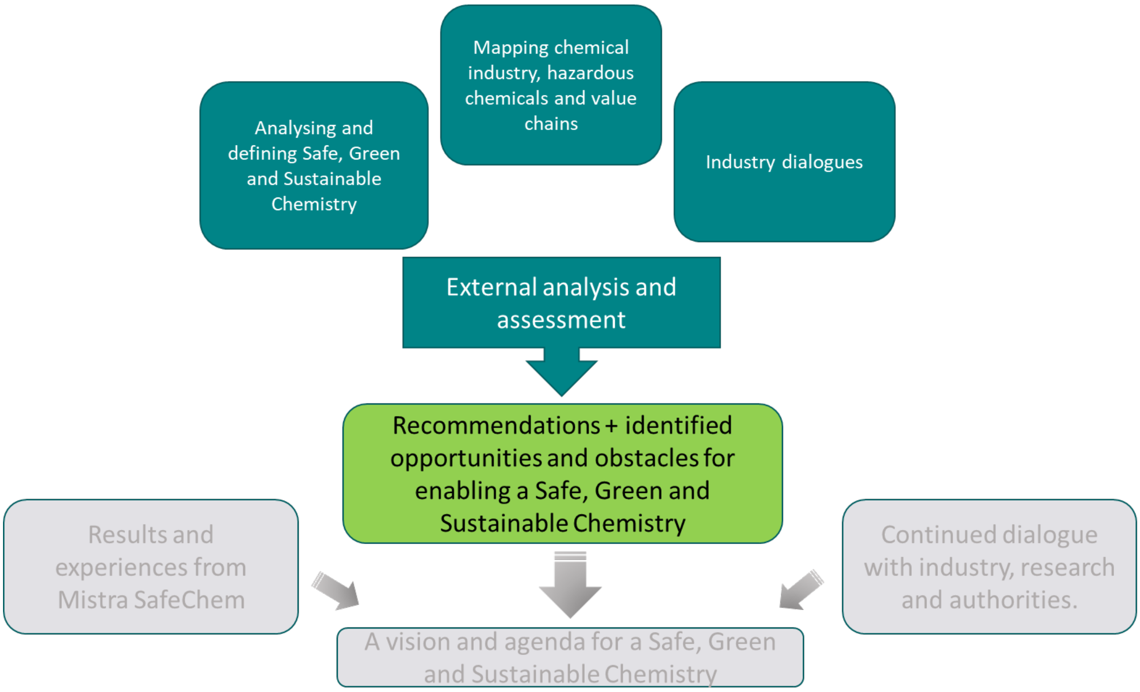

Figure 1. Schematic description of components of this report – and link to the next steps and final results (in grey). External analysis represents the collection and analysis of relevant external information from e.g. politics, industry or science that can be expected to have an influence on the transformation to a safe, green and sustainable chemistry.

A Safe, Green and Sustainable Chemistry – concepts and initiatives

Green and Sustainable Chemistry

The concept of "Green Chemistry" and its 12 principles was originally presented by Anastas and Warner (1998) and was used as inspiration for the launching of the call for proposals which resulted in the Mistra SafeChem programme. A brief description of the concept and examples of how it has been expanded and developed is presented here.

In the original definition, green chemistry was defined as "the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances" (Anastas and Warner, 1998). Green chemistry recognizes hazard as a molecular property that chemists can influence in the same way that we design molecules for colour, solubility, melting point, reactivity, etc. Hazard refers to the endangerment of humans, or other life forms, by physical danger (e.g. fire and explosions), toxicological and ecotoxicological effects – acute and chronic, including emerging issues such as endocrine disruption and epigenetic phenomena and Global deterioration – including global warming, ozone depletion, exhaustion of natural resources, acid rain, and others. The 12 principles of Green Chemistry cover a life-cycle perspective covering all stages from design and production of basic chemicals, components and products to consumption and disposal/recycling.

The concept was adopted, in slightly modified (and re-named by exchanging green for sustainable) forms by OECD (1999) "Sustainable chemistry is the design, manufacture and use of efficient, effective, safe and more environmentally benign chemical products and processes that prevent pollution, reduce or eliminate the use of hazardous waste, and reduce risk to human health and the environment." IUPAC (2000) adopted a slightly modified definition formulated as ”The invention, design, and application of chemical products and processes to reduce or to eliminate the use and generation of hazardous substances." The concept of Green Chemistry has also been expanded to Green Engineering to include a broader range of industrial activities in 12 Principles of Green Engineering[1].

In the scientific literature there are many examples of further development and discussions of the green chemistry concept and discussions of potentials for implementation (e.g. Anastas and Eghbali, 2010). A search of Web of Science[2] yielded 3 113 published articles with the words *green chemistry* in the title, most of them covering new and specific synthetic, analytical or separation processes which were developed following one or more of the 12 principles of green chemistry. Revised definitions have also been developed and include a stronger focus on circularity (e.g. Keijer et al., 2019). In addition, guiding principles and actions to be taken have been presented by Blum et al. (2017). Methods developed for setting quantitative criteria for the 12 principles of green chemistry (qualitative in the original definition) have also been presented (Martínez et al., 2022).

The Sustainable Chemistry framework is a further development of sustainable and safe chemical handing (Blum et al., 2017, Elschami and Kümmerer, 2018). The framework focuses on the deliverance of a service or function in the most sustainable way, aiming to take all sustainability dimensions into account. Compared to green chemistry it also includes non-chemical alternatives or service-based business models that need to use fewer and less chemical products. Moreover, the framework has circularity as an important aspect (ECOSChem, 2023) taking both the opportunities and the limitations of a circular economy into account.

The EU Chemical Strategy for Sustainability

On October 20, 2020, the EU CSS towards a toxic-free environment was released. The strategy aims to better protect citizens and the environment and to boost innovation for safe and sustainable chemicals. It includes an ambitious roadmap with actions for implementation.

The strategy represents a major initiative towards safer production and use of chemicals – and a better protection of human health and ecosystems from chemical pollution. It also states that chemicals are expected to contribute to the green and sustainable transition in Europe – and to the fulfilment of the global Sustainable Development Goals[3]. The CSS can thus be said to set two parallel goals - maximise the benefits of chemicals and the chemical industry while reducing the risks. A graphic summary of the strategy is presented in Figure 2.

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[1] https://www.acs.org/greenchemistry/principles/12-design-principles-of-green-engineering.html
[2] Search: performed 2023-03-06. Keywords "Green chemistry" in title-
[3] https://sdgs.un.org/goals

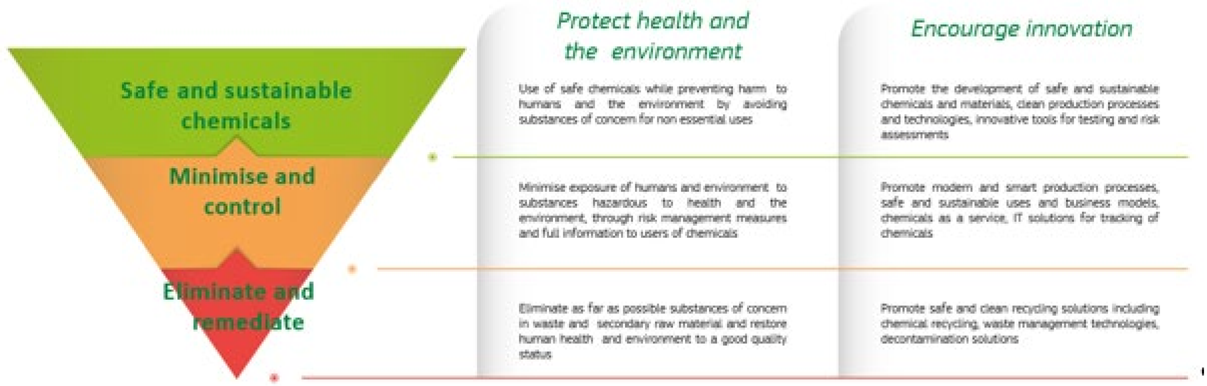

Figure 2. The Toxic-Free Hierarchy from the EU Chemical Strategy for Sustainability (COM, 2020)

The chemical strategy has many things in common with the 12 principles of Green Chemistry (Anastas and Warner, 1998) but with more focus on sustainability and a circular economy thus complementing the original concept with relevant criteria but also possibly increasing the complexity of implementation. The strategy also emphasises the role of chemicals in the Green Deal[4] and transformation to a sustainable and climate neutral EU.

The implementation plan of the strategy contains a number of critical topics which will require in-depth assessment and dialogues to arrive at transparent and relevant decisions, most notably setting criteria for “Safe and Sustainable by Design” and “Essential Use”. For long-term success of the chemicals strategy, large efforts are needed for research and innovation followed by investments in industry, and a number of projects dedicated to these topics are already underway in the Horizon Europe programme.

Essential use was introduced in the CSS but has been used, with slightly different definitions and criteria, in international conventions such as Montreal, Stockholm and Minamata (Garnett and Van Calster, 2021). REACH does not include a definition of essential uses but socioeconomic analysis under restriction and authorisation could include considerations of criticality for the functioning of society and necessity for health or safety as part of the benefits of use.

The starting point for the criteria (as established in the CSS) indicate that essentiality of a use is defined by:

1. ‘The use is necessary for health and/or safety’ AND/OR ‘critical for the functioning of society’.

and

2. There are no alternatives that are acceptable from the standpoint of the environment and health.

How these criteria should be set and how responsibilities for approving substances for essential use will be assigned is currently under discussion (see e.g. Wood E&IS GmbH – April 2022).

The CSS also includes the concept “Safe and Sustainable by Design” (SSbD) which is intended to be a framework that focusses on the design and development of safe and sustainable chemicals and

[4] https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_en

materials. SSbD covers the entire value chain and the entire life cycle and will enable the move towards zero pollution and circularity by avoiding substances with properties that may be harmful to human health or the environment. It integrates circularity, climate neutrality, functionality and safety of materials, products and processes throughout their life cycle. The Commission, through JRC, has developed criteria and procedure for evaluation of chemicals and materials with respect to SSbD (Caldeira *et al.*, 2022; European Commission, 2022). Industry is also engaged in this issue and have proposed a methodology for assessment (Cefic, 2022). The proposed assessment methods vary in approach and complexity but have in common a life cycle approach and assessment of hazards and risks for exposure in the value chains of products and materials. A simplified approach, entirely based on the hazard properties of chemicals used, has also been proposed by the NGO Chemsec (2022).

The development and implementation of a common SSbD methodology will require continued efforts involving the research community, industry, authorities and civil society to ensure the applicability, relevance and acceptance. Activities to reach this are also underway in research programs such as PARC[5] and IRISS[6] (see below).

Industry initiative on chemicals and sustainability

SusChem is the European technology platform for sustainable chemistry. It is a forum that brings together industry, academia, policy makers and the wider society with a vision for a competitive and innovative Europe where sustainable chemistry and biotechnology together provide solutions for future generations. SusChem aims to initiate and inspire European chemical and biochemical innovation to respond effectively to societal challenges by providing sustainable solutions. SusChem secretariate is based at CEFIC, with national platforms in 17 countries including Sweden: www.suschem.se.

As a part of defining the future potential global benefits of the chemical industry, SusChem has evaluated societal challenges related to the UN Sustainable Development Goals (SDG) and how the chemical industry can potentially contribute to overcome them. A summary of this evaluation and the role of the chemical industry is presented in Table 1 below. For a full description, see www.suschem.org/un-sustainability-goals-1

Table 1. The beneficial contributions of the EU chemical industry to Sustainable Development Goals. Summarised from www.suschem.org/un-sustainability-goals-1

Sustainable Development Goal	Summary of the role of the chemical industry
Zero Hunger	… more efficient and sustainable production methods …
Good Health and Wellbeing	… greater efforts are needed to fully eradicate a wide range of illness and better support our ageing population.
Clean Water and Sanitation	… water purification technologies and advanced water management systems that can ensure safe and affordable drinking water and adequate sanitation for all.
Affordable and Clean Energy	… sustainable solutions to boost the use of renewable energy and develop energy storage markets …improve energy efficiency.

[5] https://www.anses.fr/en/content/european-partnership-assessment-risks-chemicals-parc
[6] www.iriss-ssbd.eu

Industry, Innovation and Infrastructure	Sustainable innovation is the basis for transport, irrigation, energy and environmentally sound industrialisation …. inclusive economic development.
Sustainable Cities and Communities	… sustainable chemistry provides a toolbox of key innovations that enable energy and resource efficiency, smarter buildings and mobility in our future cities.
Responsible Consumption and Production	… improving resource and energy efficiency along its value chains and contributing to the development of a circular economy.
Climate Action	… has an essential role in the development of advanced materials and effective technologies for renewable energy production and storage.

SusChem has also presented a Strategic Research and Innovation Agenda (SRIA) (SusChem, 2020) where three main challenges; Circular economy and resource efficiency, low-carbon economy towards mitigating climate change, and protecting environmental and human health are discussed along with a comprehensive documentation of research and innovation needs in areas such as advanced materials, advanced processes and enabling digitalisation. Specific sections are dedicated "Sustainability Assessment Innovation" and "Safe-by-Design for Chemicals and Materials". In these sections, many of the research topics in focus in Mistra SafeChem are highlighted such as Tools for prospective sustainability assessment, Framework for recommended methodologies and structures on early-stage and semi-quantitative assessments, A functional approach for safe-by-design and Minimising toxicity in combination with overall sustainability improvements (full life cycle perspective).

Defining a Mistra SafeChem concept for Safe, Green and Sustainable Chemistry

In Figure 3, a simple illustration of the Mistra SafeChem concept of Safe, Green and Sustainable Chemistry is presented. This concept, although not illustrating the complexity of the challenges involved nor the advanced research required to overcome these challenges, provides a framework where all components of the research performed in the programme can be represented. The concept should thus not be considered as a new and further developed version of the original concept and it´s more recent additions but rather a concept for illustration and visualisation of main components and challenges. The concept will also be used to structure the final programme synthesis and the formulation of a vision and agenda.

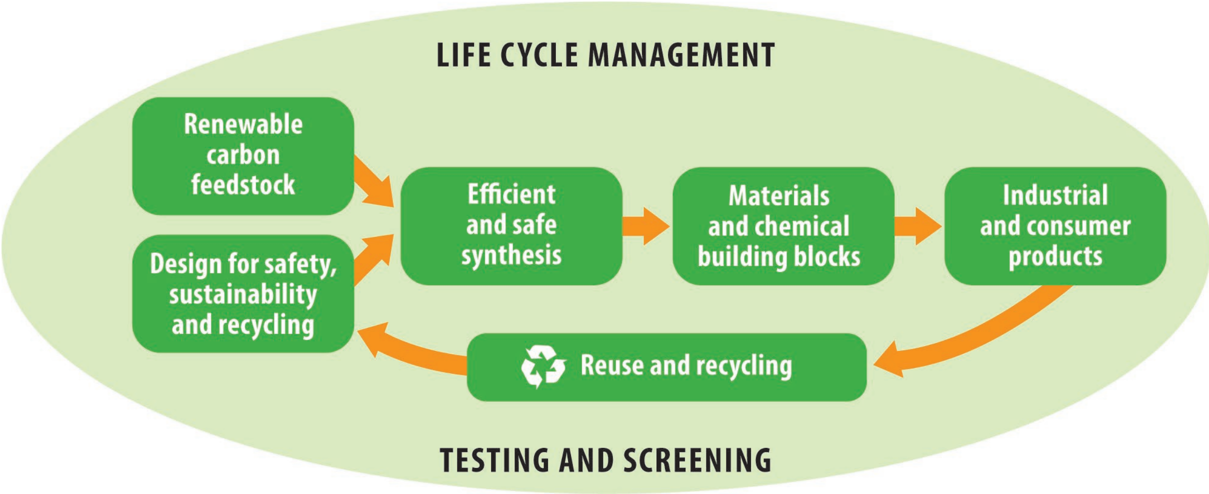

Figure 3. A simple concept for Green Chemistry in Sweden – and a framework to illustrate how the research performed in Mistra SafeChem contributes

The green boxes in the concept illustration can be described as representing a safe, green and sustainable value chain but also the research activities in the programme where novel chemical synthesis steps are developed and, in some cases, using renewable (wood based) and recycled (textile) materials. The life cycle management covers all steps in the value chain both in the illustration and in terms of the research in the programme – LCA is applied also in very early design stages and includes novel impact assessment methods covering both chemical exposure and risks. The same is true for testing and screening, where the research is focussed on development of *in silico* and *in vitro* methods for toxicity assessment and hazard screening which can be applied in all steps of the life cycle of a chemical, material or product. The Mistra SafeChem programme was designed prior to the release of the EU Chemicals Strategy for Sustainability and the above described industry initiatives for sustainability but many of the research components of the Mistra SafeChem programme will potentially support the development and implementation of these.

The main contributions from the Mistra SafeChem programme include tools for hazard and risk screening and life cycle assessment as well as new synthesis processes of relevance for future production of chemicals.

Mapping of chemical industry, chemicals and value chains in Sweden

The chemical industry in Sweden

Scope and approach

To make an assessment of how to promote and expand green chemistry in Sweden, it is important to first understand what the chemical industry in Sweden looks like.

First off, the chemical industry is traditionally defined as the companies that produce industrial chemicals and consumer products. However, overlaps often exist with other sectors such as the plastic industries and pharmaceutical industries that also produce molecules of various kinds.

To get a better understanding and overview of the chemical industry, Vinnova financed a study in 2016 where an extensive mapping of the Swedish chemical industry was conducted (Mossberg, J., 2016). This study was based on statistical data from Statistics Sweden (SCB). To ensure the correctness and quality of the data, it was assessed by a panel of experts. In the study, companies belonging to the business segments refining, biorefining, basic chemicals, chemical products and pharmaceutical products were analysed based on their number of employees, type of activity (production, business, research and development (R&D)), location and other characteristics). About 515 companies were covered – out of which roughly 440 were active in 2014, which was the year the data in the report were based on. Companies involved only in sales, marketing and/or transport of chemical products were not included, neither was manufacturing of plastic products.

Results

Some of the graphs and tables presented in the 2016 report are shown below in Figures 4 to 6. Collectively they give an overview of the types of chemical companies active in Sweden in 2014.

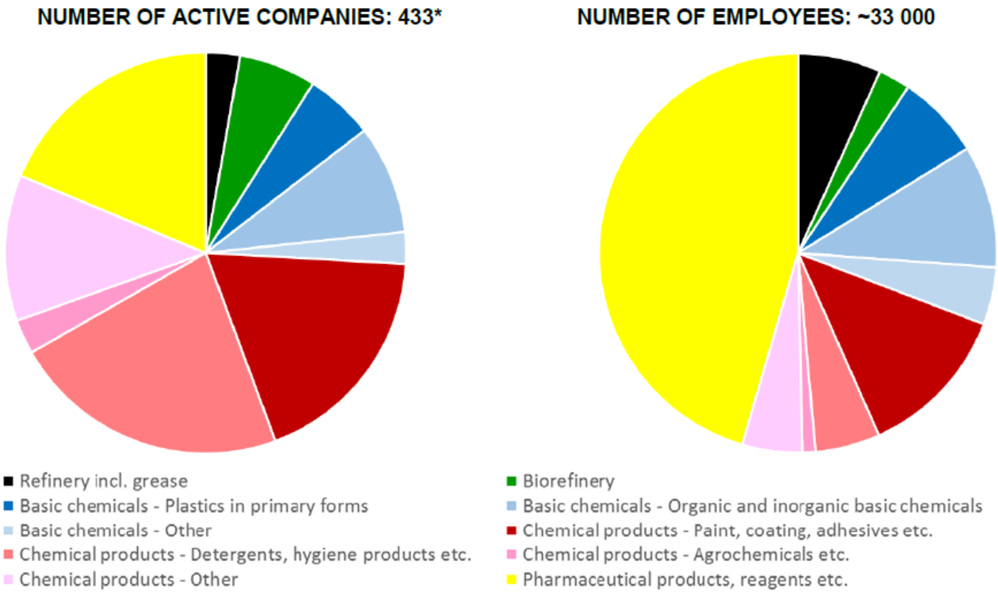

Figure 4. The chemical industry in Sweden 2014 divided by companies and employees in the different business segments (Picture from Mossberg, J. 2016. Reprinted with permission.)

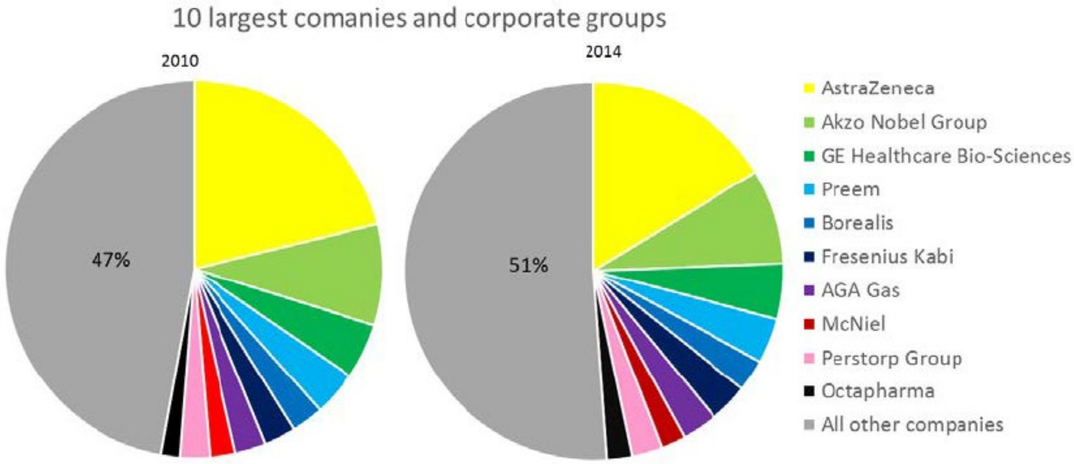

Figure 5. The ten largest companies and corporate groups and their share of total employment (Picture from Mossberg, J. 2016. Reprinted with permission)

Looking at individual companies it could be seen that Sweden is dominated by a limited number of large companies and corporate groups and 15% of the companies account for 80% of the employees. The ten largest companies and corporate groups account for 49 % of the employees, AstraZeneca and the Akzo Nobel group (nowadays split between AkzoNobel and Nouryon) being the two largest employers. Five of the ten largest companies are from the business segment pharmaceutical products.

Economic analyses were also made in the report. Pharmaceuticals stand for approx. 33% of the export values of chemicals, again highlighting the size and importance of this business segment in Swedish chemical industry.

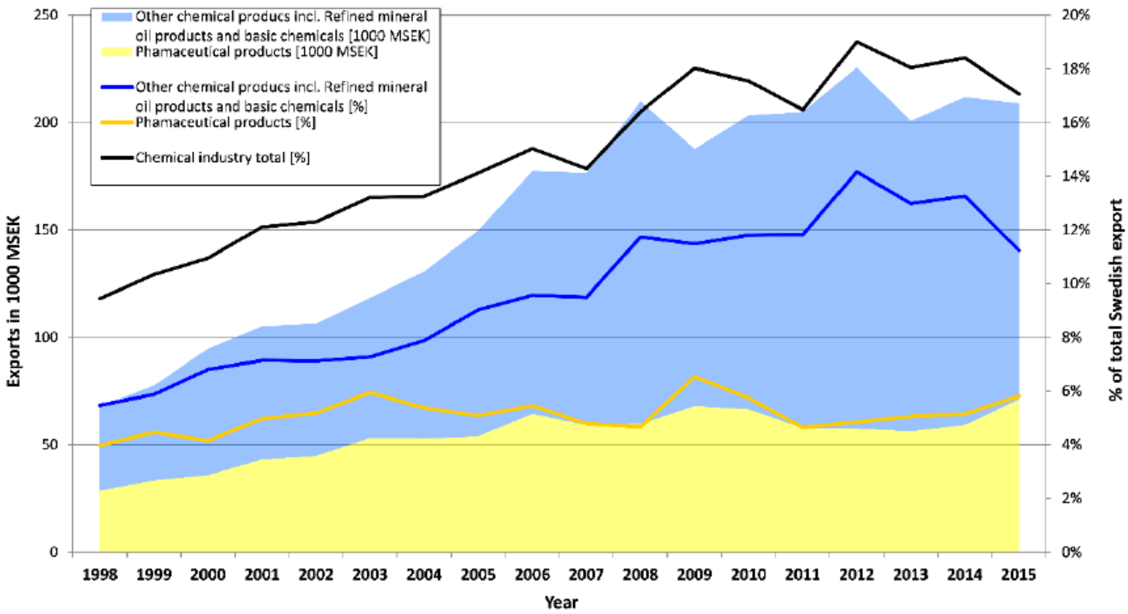

Figure 6. Aggregated export data for products produced by the chemical industry years 1998-2015. The stacked area shows the absolute exports in 1000 MSEK (left axis) and the lines show the exports in relation to total Swedish exports in % (right axis). Yellow represents pharmaceutical products, blue represents other chemical products (the black line represents the chemical industry total) (Picture from Mossberg, J. 2016. Reprinted with permission)

Overall, the report from Mossberg (2016) clearly illustrates the complexity in defining "chemical industry in Sweden" with a large variation in size and production capacity, dependence on import/export on a global market and with a variety of value chains involved. One conclusion from the report (not pictured in a graph) was that apart from companies in the business segment "Pharmaceutical products, reagents, etc.", the majority of companies are focused on production. Hence, only very few of the companies have product development and R&D activities in Sweden which is the business functions where and an impact on the design process of new chemicals and materials can be made.

Volume and characteristics of chemicals produced and used in Sweden

Scope and approach

All manufacturers, importers and sales agents need to report their chemical products (and biotechnical organisms) to the Swedish Chemicals Agency's Products Register. The registration covers information such as hazard statement, labelling, function of the product, sector of use, composition, ingoing substances, quantity data and sales values. The Products Register thus represents a large information source which potentially can be used to evaluate trends and patterns in production and use of chemicals in general, or for specific groups of chemicals. Another possible use is to identify groups of chemicals where there is a potential need to further assess risks and take action to minimise these risks. This in the perspective of a safe, green and sustainable chemistry as well as to precede future regulations and implementation of the EU Chemical Strategy for Sustainability.

The data in the Products Register are classified with GHS-codes (Globally Harmonized System of Classification and Labelling of Chemicals) that represent the inherent hazards of a chemical and with these different hazard classes follow requirements of marking, labelling and packaging. While the classification with GHS-codes does not provide information on risks associated with use or handling of the chemicals, it can be used as a first indicator for prioritisation of candidates for further investigation and potential substitution when pursuing a shift to a safe, green and sustainable chemical industry.

The data in the Products Register is to a large extent confidential for reasons of market competition. Access to this data for research or evaluation is thus only possible in aggregated form where individual market actors cannot be identified.

For this study, the Swedish Chemicals Agency provided an extract from the Products Register for 2019 with information about functional codes, labelling with GHS-code, number of products and quantity of the product. Another extract received coupled the functional codes to the sector of use together with numbers and quantities of the products. Functional codes describe the technical function of the registered chemical, e.g. binder, antioxidants, detergents, chelating agents. A maximum of four functional codes can be added in the register for a certain product. The data were divided among what is produced in Sweden on one hand and what is imported from other EU countries or countries outside the EU on the other.

By combining this information, it was possible to map different industry sectors use of products labelled with health hazard (GHS08) or environmental hazard (GHS09). The pictograms of the hazard classes that require a product to be labelled with GHS08 and GHS09 are shown in Figure 7 and presented in more detail in Appendix I.

Figure 7. Pictograms for health hazard (GHS08) and environmental hazard (GHS09)

Results

For the products label with “serious health hazards” and “hazardous to the environment” the tonnage of production and use the manufacturers or importers have registered per sectors of use is summarized in Figure 8 and 9 (worth noticing is that the production and import of petroleum products have been excluded from the survey, as the purpose has been to study rather the use of chemicals in industries rather than fuels).

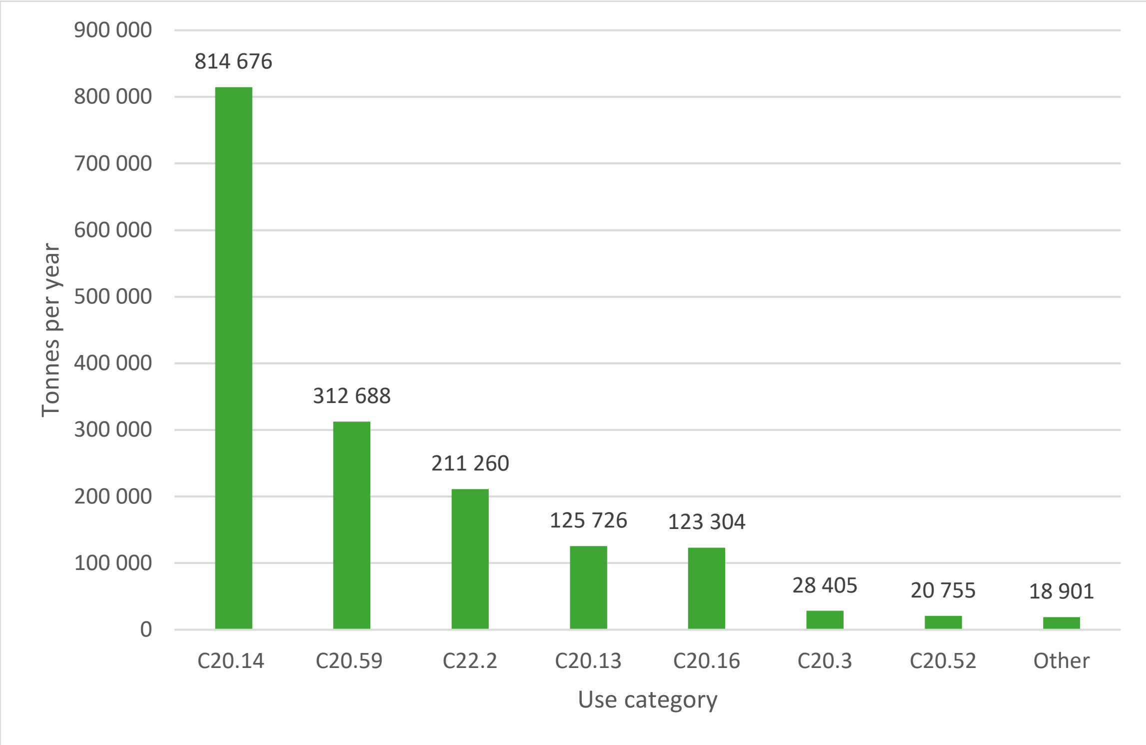

Figure 8.1 Total production/use - compounds with classification Serious health hazard (08). Use categories illustrated in individual bars represent: C20.14 - Manufacture of other organic basic chemicals; C20.59 - Manufacture of other chemical products n.e.c.; C22.2 - Manufacture of plastic products; C20.13 - Manufacture of other inorganic basic chemicals; C20.16 - Manufacture of plastics in primary forms; C20.3 - Manufacture of paints, varnishes and similar coatings, printing ink and mastics; C20.52 - Manufacture of glues

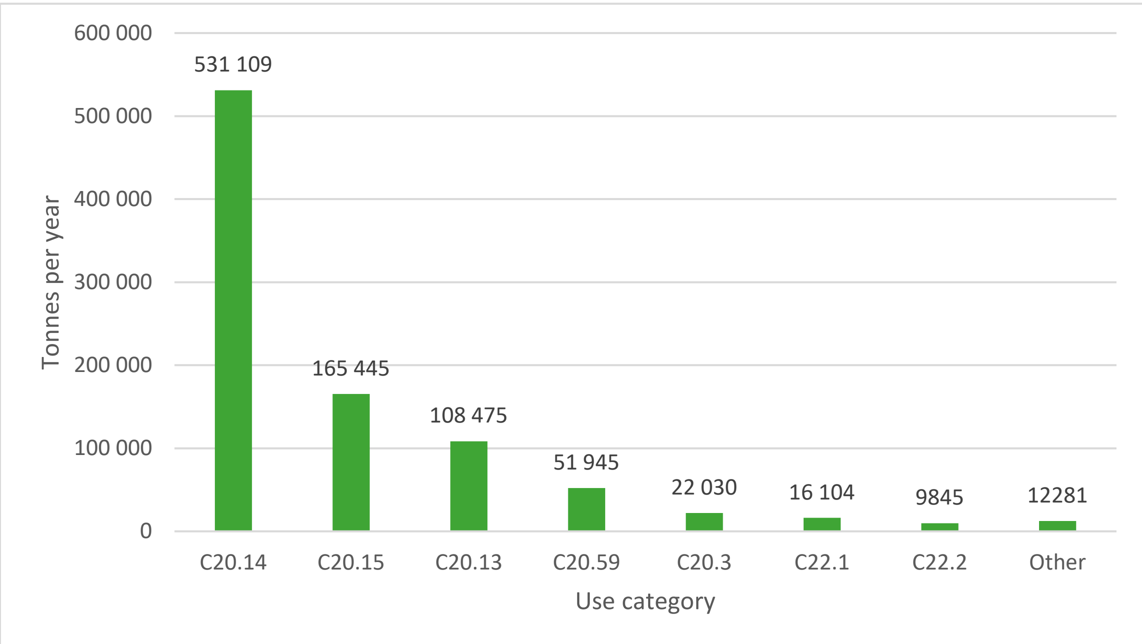

Figure 9. 2 Total production/ use - compounds with classification Hazardous to the environment (09). Use categories illustrated in individual bars represent: C20.14 - Manufacture of other organic basic chemicals; C20.15 - Manufacture of fertilizers and nitrogen compounds; C20.13 - Manufacture of other inorganic basic chemicals; C20.59 - Manufacture of other chemical products n.e.c.; C20.3 - Manufacture of paints, varnishes and similar coatings, printing ink and mastics; C22.1 - Manufacture of rubber and plastic products; C22.2 - Manufacture of plastic products

The three main sectors where larger amounts of products with serious health hazards (GHS code 08) are used are:

- Manufacture of other organic basic chemicals
- Manufacture of other chemical products[7]
- Manufacture of plastic products

The three main sectors where the highest use of chemical products that are hazardous to the environment (GHS code 09) are used are:

- Manufacture of other organic basic chemicals
- Manufacture of fertilisers and nitrogen compounds
- Manufacture of other inorganic basic chemicals

With the functional codes for the chemical products, it is possible to get an overview of what functions the chemicals used in a specific sector may have. For C20.14 Manufacture of other organic basic chemicals the functions raw materials and intermediates, process regulators and binding agents counts for the largest amounts. By then checking occurring labelling of chemicals registered with specific functional codes it shows that for example binding agents may be labelled either hazardous to the environment or with serious health hazard. It could hence be of interest to investigate the different chemicals registered under a functional code (e. g. binders) to find out if there are less hazardous alternatives that may replace more hazardous chemicals with the same function.

For further understanding of the use of chemicals within Swedish industry it is suggested to study in detail which sectors are using functionality chemicals that are hazardous. Such a study needs to go deeper than labelling to understand the identity of the chemicals. Provided it is possible to get data from the Products Register also on CAS-number level it would be possible to identify candidate chemicals that might be substituted to less hazardous alternatives or uses that may be subjected to development of alternative processes/products providing the desired function.

From the data from the Products Register it is clear that it will be important to further study risk reduction potential for the large group with the function raw material and intermediates produced in Sweden, where 318.284 tonnes were labelled hazardous to the environment and 473.382 tonnes labelled with serious health hazard. For chemicals imported into Sweden this category is by far the largest. Other imported functional groups that may be studied are binding agents, process regulators and lubricants.

[7] This class includes manufacture of photographic plates, films, sensitised paper and other sensitised unexposed materials- manufacture of chemical preparations for photographic uses- manufacture of gelatine and its derivatives- manufacture of various chemical products: • peptones, peptone derivatives, other protein substances and their derivatives n.e.c. • chemically modified oils and fats • materials used in the finishing of textiles and leather • powders and pastes used in soldering, brazing or welding • substances used to pickle metal • prepared additives for cements • activated carbon, lubricating oil additives, prepared rubber accelerators, catalysts and other chemical products for industrial use • anti-knock preparations, antifreeze preparations • liquids for hydraulic transmission • composite diagnostic or laboratory reagents

Industry dialogues

Scope and approach

Through interviews with representatives from the chemical and chemical handling industry and following the ongoing discussion in Sweden and abroad, several valuable inputs on opportunities and obstacles connected to safe, green and sustainable chemistry have been received. These points are presented in Table 2 and constitute both technical issues, such as the need to assess and evaluate chemicals and material, and economic and political incentives that are required for to take further steps in creating a safe, green and sustainable chemical industry. It should be noted that this is based on communication with a limited number of industrial representatives and the responses have been edited and summarized by the authors of this report.

Table 2 Outcome from interviews with representatives from the chemical and chemical handling industry. Summarized and edited by the authors into the three categories opportunities, challenges and requirements.

Topic	Opportunities	Challenges	Requirements
Production of chemicals	Stakeholders communicated that opportunities are increasing for frontrunners that are first on the market with environmentally sustainable products. More opportunities are available for moving away from hazardous and problematic substances. One example is the move from traditionally used scarce metals in the palladium group to more abundant 1st row metals such as iron, copper, or nickel catalysts, and also the increased knowledge in enzyme catalysis.	Hazard and toxicity assessment must be speeded up, cost less and results be more reliable (connect to regulatory compliance) to take multimillion investment decisions. Access to competitive "green material", e.g. non-fossil based materials, might be an obstacle. Many actors highlight that the majority of "interesting" biobased compounds today are used as fuel. The investments needed for handling new types of chemicals and materials are high. Even though sustainable products have a market, there are still several examples of where customers are not ready to pay the "green" premium fee.	The industry needs to have access to better tools that can make hazard, risk, and life cycle assessment cheaper and faster. Support (financial, infrastructure, regulations and policy, taxonomy regulations) from the state and EU for green solutions. Ensure that green and sustainable chemistry is included in the education of tomorrow's students to be able to hire staff with the right competence. Sweden and the EU should continue facilitating the supply of biobased raw materials, CCU (Carbon Capture and Utilization) or utilization of biomass.
Production of products containing chemicals	Many producers in value chains have substance list and restriction lists, often moving ahead of regulations. Good starting point for substitution and aid in material choice. EU CSS can hopefully clarify what safe and sustainable is. This can help prioritization of industry activities.	EU CSS is a good initiative, but alignment globally will be needed to help global companies to be efficient. Assessment of sustainability is very complex due to the limited possibility to get all relevant product data from supplier during the development phase.	Further refined tools that help in making safe substitution that take all sustainability aspects into consideration: climate change, human health effects and costs etc. Easy-to-use tools and guidelines that can aid in decision making when comparing alternatives with different chemical compositions.
Use of biomass for production of chemicals and materials	The EU CSS and increased focus on circularity makes the demand for biobased chemicals high.	Producers relying on biobased materials cannot risk a batch-to-batch changes or a shortage.	Better tools, more data and increased competence for hazard, risk and environmental assessment fit for biobased chemicals and materials.

Trends observed

In the dialogues with the selected stakeholders some general trends were observed. First, assessments on safety and sustainability are conducted already in the design phase, meaning that the actors saw the need to make these assessments as early as possible in their innovation or development process. However, several challenges were identified in terms of data availability, the cost for making the assessment (both time spent delaying product launch and actual costs) and the reliability of the assessment for taking larger business decisions.

Moreover, the main focus for most companies is reduction of greenhouse gas emissions with most interviewed actors having climate ambitions in line with the Paris Agreement[8]. This seems to be a strong driver in the chemical industry and focus is put on minimizing CO_2-footprint and evaluating possibility to switch to biobased feedstock. Not as harmonized, but also communicated in the interviews as becoming more important. is to set targets on other environmental aspects such as water use, prevention and reduction of waste and lowered effect of ecotoxic and toxic substances.

In discussion about changes in regulations, it became clear that the industry is not against new regulation, quite opposite they welcome it since it makes the rules clearer. However, the companies ask for more support in assessing and approving new types of compound classes or material when others are prohibited.

Chemicals in the value chain of products

When reviewing the obstacles and opportunities linked to green and sustainable chemical industry it is important to remember that chemical value chains are complex, and chemicals are used in all sectors of society. A specific chemical can be produced and then used in a variety of value chains as a building block for additional molecular synthesis, as industrial reagents, additives to materials or as a main component of consumer products. This makes chemical value chains difficult to characterize, especially in view of allocating benefits and potential hazards and risks to a large number of steps in life-cycle based assessments of value chains or multiple uses of specific chemicals.

Adding to this complexity is the lack of, or unavailability of, information on specific chemicals in any value chain. With complex value chains, including many actors and covering international or global markets with different chemical regulation and control, obtaining accurate information on composition of chemical products or materials can be a challenge for industrial actors towards the end of the value chain. Without accurate information, the possibilities for an industry actor towards the end of the value chain to influence the development of safe alternatives and thus embark on a transformation journey to green and sustainable chemistry is limited. Likewise, for a producer of a chemical with multiple uses in complex value chains, it is difficult to have control and information on all potential uses of this chemical and to accurately assess both potential chemical risks and sustainability. Collaboration within the different value chains where chemicals are produced, converted or used in materials, as components in products is crucial.

These challenges are also addressed on the European level. An on-going EU funded project *IRISS – The international ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes*[9] () has the aim to connect, synergize and transform the SSbD community in Europe and globally. Within IRISS, an assessment of the challenges with implementing the safe-and-sustainable-by design concept is being conducted for seven value chains (on European level). The identified challenges within these value chains will be related to both implementation of green and sustainable chemistry during production of the materials and to difficulties in end-of-life treatment of the products.

In IRISS, a first definition of challenges was made in dialogue with industry representatives of these seven value chains (packaging, textile industry, construction, automotive industry, energy materials, electronics and fragrances). Challenges common to the value chains were related to e.g. availability of biobased and recyclable raw materials (including critical raw materials), depletion of natural resources and avoiding significant climate impacts. Risks and/or safety related to chemical exposure

[8] https://unfccc.int/process-and-meetings/the-paris-agreement
[9] www.iriss-ssbd.eu

of humans and the environment were mentioned specifically by the value chains of packaging, textile industry, the automotive industry and electronics. In addition, the complexity of global value chains was mentioned in relation to both chemical and component traceability and control over occupational health and basic labour rights abroad.

Conclusions and outlook

This purpose of this report is to summarise the results of a set of initiatives taken to identify opportunities and obstacles for enabling a safe, green and sustainable chemical industry. It represents a mid-term result in the work aiming to present a final vision and agenda for green chemistry in Sweden. The conclusions and outlook presented below are the result of initial activities including mapping of chemical industry and production and use of chemicals, industry dialogues and external analysis.

Opportunities

- The concept of *Green Chemistry,* including its different versions developed after the original definition, is still relevant and can provide a framework for enabling the transformation towards a safe, green and sustainable chemical industry. There is also vast experience from research and innovation performed with green chemistry principles that can provide inspiration and guidance. A simplified concept has been developed in the Mistra SafeChem programme and is used as a common concept to frame and define how the different research components of the programme contribute to its overall aims and vision.

- Further strengthening the ideas behind the *Green Chemistry* concept, the launching of the EU Chemical Strategy for Sustainability provides a strong and coordinated opportunity to develop the European chemical industry and the societal use of chemicals in a *green and sustainable* direction and to contribute to the green transition. As part of this, the development of the SSbD framework (Caldeira et al., 2022) will help boost the development and implementation of early safety and sustainability assessment of chemicals and materials.

- Industry initiatives demonstrate the same high ambition level further strengthening the possibilities to achieve actual change. As made clear from discussion with several stakeholders both inside and outside of Mistra SafeChem there is an ever-increasing focus on safety and sustainability. This to be compliant with existing and upcoming regulations, and also to be able to meet market demands for "green" products with specific and declared properties.

- Research, innovation and investments are central to the future development. Linked to the EU Chemical Strategy for Sustainability, research funding within the Horizon Europe program has also been directed to specific challenges and knowledge needs such as definition and development of methods to operationalize SSbD concept, and innovative production processes, chemicals and materials.

- Industry dialogues reveal that the market demand for products that are both biobased and safe is getting stronger and stronger. This is pushing industry frontrunners towards finding new application for material from biobased and renewable sources.

- To further map the use of chemicals within different Swedish industry sectors, data from the Products Register also on CAS-number level together with hazard classes could make it possible to identify candidates for substitution to less hazardous chemicals.

Obstacles

- Chemical value chains are complex, international/global and include all societal sectors. Mapping chemical production and use with the purpose of analysing risks and prioritising areas for action/development is thus difficult and involves many actors. Utilising central databases on chemical import/export and use such as the Swedish Products Register might be a way forward.

- It is hard to find both the individual companies selling and using hazardous chemicals. With data from the Products Register it is possible to identify industry sectors using hazardous chemicals, but the names of the individual companies selling the products are confidential and the users are not obliged to register their uses with the Products Register. It is hence difficult to find the actual downstream users using the data at hand. However, industry associations may be a way to communicate with downstream users.

- The chemical industry is a heterogenous group of companies with main activities ranging from small scale production of speciality chemicals, pharmaceutical industry to large-scale production of base chemicals for a variety of applications and value chains. Different parts of the chemical industry also have widely differing conditions in terms of markets and market competition, industrial infrastructure, financial strength which all affect the possibility for change and introduction of new green and sustainable production methods and products.

- A shift to renewable energy and biobased raw materials is the highest priority for many industries. To avoid introducing new chemical hazards and risks when implementing solutions for the climate challenge, assessment of potential chemical risks in new production processes, new chemicals and materials is necessary.

- The development of reliable and low-cost tools for assessment of chemical hazards of innovations, new chemicals or materials, taking into account potential hazards and risks in a life cycle perspective is urgently needed to facilitate response to market demands of safe and sustainable products.

- To truly push for change, regulating bodies should aim to ban known problematic substances faster. As of now, front running companies are cautious to develop replacements since problematic compounds such as per- and polyfluoroalkyl substances (PFAS) and phthalates can be allowed for decades even though the health and environmental issues have been demonstrated.

Relevance of Safe, Green and Sustainable chemistry to industry and society

The general principles of a safe, green and sustainable chemistry are applicable to all industry sectors and to all use of chemicals in society. There are, however, areas where a future implementation of these principles will require further dialogue and decisions on definitions, methodology and applicability. This is particularly evident for the future implementation of principles for SSbD and Essential use. Two additional topics where continued research and development needs to go hand-in-hand with dialogues between societal actors are:

- **Risk or hazard?** While the original concept of Green Chemistry focuses on reduction use of hazardous properties of chemical compounds, later developments have introduced a risk management perspective i.e. not eliminating hazard but focussing on minimizing risks associated with exposure. Similarly, the concepts proposed for SSbD range from being based entirely on the hazardous properties of the chemicals or a risk-based approach.

- **Industries that intentionally produce biologically active substances**. The pharmaceutical industry produces compounds that are intentionally biologically active and, in many cases, have hazardous properties that can lead to negative environmental and human health impacts if not managed safely. This implies that the guiding principles of green chemistry cannot be fully implemented in terms of end-product characteristics, however, they are still relevant for guiding other steps in the value chain such as the raw material supply, production methods and waste management.

- **Renewable feedstock**. A key challenge for the chemical industry is to replace current fossil-based feedstock with biobased and renewable raw materials as one part of achieving a low carbon or climate neutral production. The potential to use forest residues or other biomass as a source of biogenic carbon has a high priority in industry and is an important aspect of a safe, green and sustainable chemical industry. While there are very large research and innovation activities underway to produce chemicals and new materials from forest biomass, there are still uncertainties in how much biomass the forest can produce with intact long-term sustainability and also how large fraction of the total feedstock that can be made available for new applications in the chemical and material industry. Another emerging opportunity for circularity is bio-CCU (Carbon Capture and Utilization) where carbon dioxide from combustion processes using biobased feedstock as fuel is captured and converted to *i.e.* methane or other base components. Although this topic is not a defined research area in the Mistra SafeChem programme, the new tools and processes being developed can be applied to ensure that the introduction of new production processes and new chemicals based on renewable biomass do not introduce new chemical risks in terms of reagents, additives, by-products or by the new chemicals and materials themselves.

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Appendix I

Table A. *Hazard classes related to human health and required to be labelled with GHS 08.*

Hazard statement	Hazard class and category
H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled	Respiratory sensitisation, Category 1 and subcategories 1A and 1B
H340: May cause genetic defects (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Germ cell mutagenicity, Category 1A, 1B
H341: Suspected of causing genetic defects (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Germ cell mutagenicity, Category 2
H350: May cause cancer (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Carcinogenicity, Category 1A, 1B
H351: Suspected of causing cancer (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Carcinogenicity, Category 2
H360: May damage fertility or the unborn child (state specific effect if known) (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Reproductive toxicity, Category 1A, 1B
H361: Suspected of damaging fertility or the unborn child (state specific effect if known) (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Reproductive toxicity, Category 2
H370: Causes damage to organs (or state all organs affected, if known) (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Specific target organ toxicity after single exposure, Category 1
H371: May cause damage to organs (or state all organs affected, if known) (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Specific target organ toxicity after single exposure, Category 2
H372: Causes damage to organs (state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Specific target organ toxicity after repeated exposure, Category 1
H373: May cause damage to organs (state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)	Specific target organ toxicity after repeated exposure, Category 2
H304: May be fatal if swallowed and enters airways	Aspiration toxicity, Category 1

Table 3. Hazard classes related to environmental effects required to be labelled with GHS09.

Hazard statement	Hazard class and category
H400: Very toxic to aquatic life	Short-term (acute) aquatic hazard, Acute 1
H410: Very toxic to aquatic life with long lasting effects	Long-term (chronic) aquatic hazard, Chronic 1
H411: Toxic to aquatic life with long lasting effects	Long-term (chronic) aquatic hazard, Chronic 2

About Mistra SafeChem

Mistra SafeChem is a research programme with the vision
to enable and promote the expansion of a safe, sustainable, and green chemical industry.

The programme is developed with the twelve principles of green chemistry as a fundament.

The research combines the potential of innovative manufacturing processes,
tools for hazard and risk screening, and life cycle assessment
with ambitions and opportunities for the development and growth
of a safe and sustainable chemical industry.

More information:
News from the programme, publications, and persons to contact
you find at the website
mistrasafechem.se

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