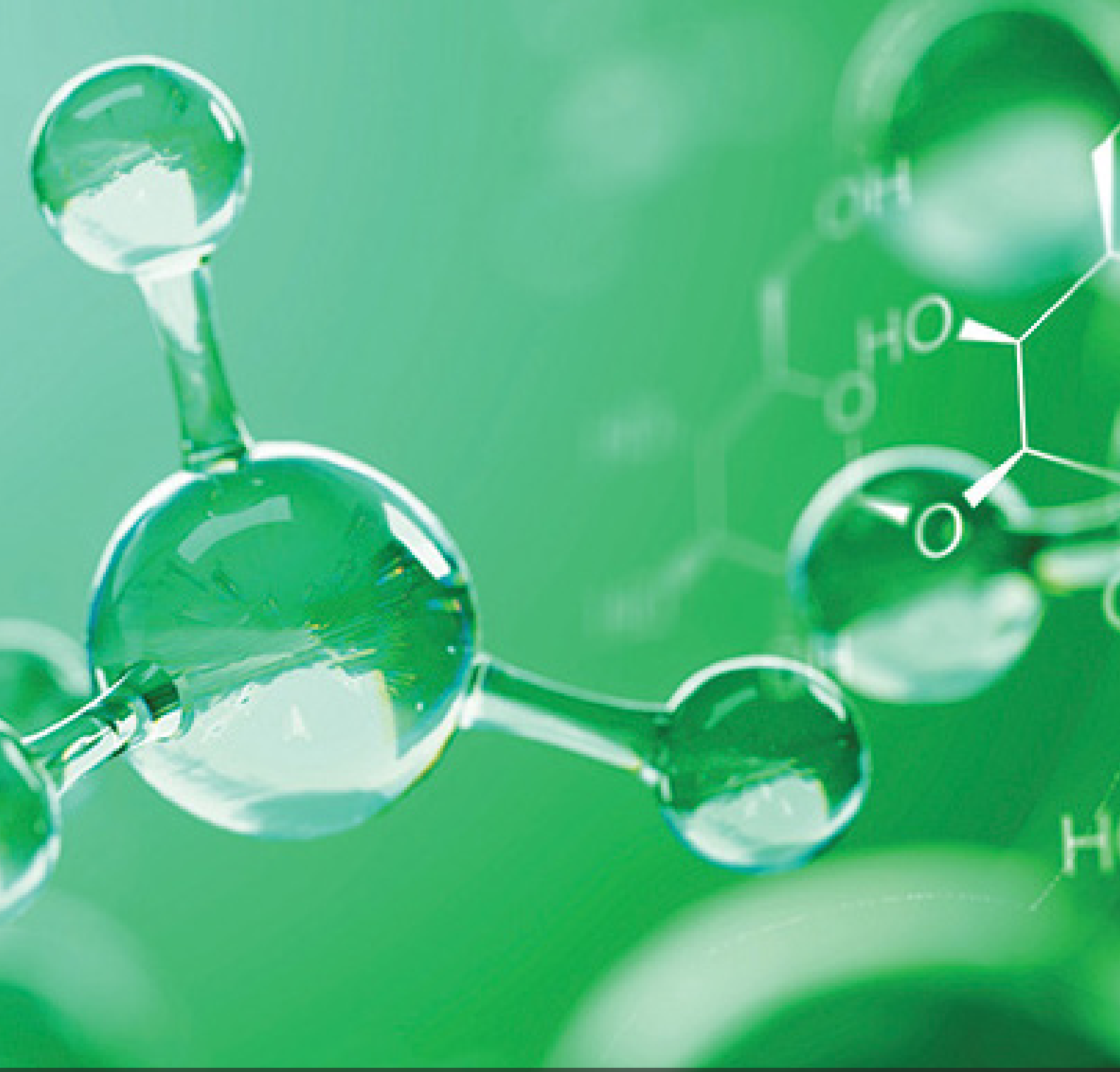

2020 ANNUAL REPORT MISTRA SAFECHEM

FUNDED BY
MISTRA
The Swedish Foundation for Strategic Environmental Research

MISTRA SAFECHEM

CONTENT

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The Swedish Foundation for Strategic Environmental Research

This is the first annual report from Mistra SafeChem,
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Alejandro Valiente (pages 10-11, 14, 23), Volvo Cars (page 18).

MISTRA SAFECHEM

The vision of Mistra SafeChem is to enable and promote the expansion of a safe, sustainable and green chemical industry

PARTNERS

Krister Holmberg,
chairman of
the Mistra SafeChem board

THE CHAIRMAN OF THE BOARD

A large and complex programme for a healthy chemical future

Starting a large research programme in the middle of a pandemic is a challenge. The kick-off, which is usually an important event where a programme culture can be implemented and researchers from different organizations can get to know each other, was replaced by virtual meetings – definitely not the same. The start of the programme was delayed but when it finally took off, the wheels seem to have been spinning smoothly. All work packages were quickly up and running, which is a sign of excellent management skills.

Mistra SafeChem is a large programme, in monetary terms the largest of all Mistra programmes to date. For the period 2020-2024, the budget is at least 100 MSEK, out of which Mistra's contribution is 70 MSEK.

It is also complex in that it engages researchers from IVL Swedish Environmental Research Institute, different units of RISE, seven university departments, of which one Danish, and no less than twelve industry partners, including some from outside Sweden. It is a demanding task for the management team to keep all this together and working towards a common goal. It is also a major responsibility for the board to secure that such a big investment in research and knowledge generation becomes successful.

The work within Mistra SafeChem covers a lot of ground. Novel, environmentally benign chemical processes will be investigated and improved methods for assessment of health and environmental aspects of chemicals will be developed.

Much of the work is of regular academic character intended for publication in good scientific journals; however, a considerable part of the budget is allocated for development work together with participating companies. Such joint projects are targeting specific issues where the health or environmental impact of chemicals is a known problem. Several case studies are already up and running and there will be more in the future.

The ultimate goal is that at the end of the programme the impact of chemicals on humans, animals and the environment will be reduced compared to today's situation. The board hopes that Mistra SafeChem will contribute to putting Sweden in a leading position in this important development.

Krister Holmberg
Professor Emeritus
Chemistry and Chemical Engineering,
Chalmers University of Technology

ABOUT THE PROGRAMME

The goal for Mistra SafeChem is a safe and green chemical industry

Mistra SafeChem is based on the concept of green chemistry and has the overarching vision to enable and promote the expansion of a safe, sustainable and green chemical industry in Sweden. Through research and development, the programme aims to reduce hazardous chemical exposure of the human population and the environment. Key features are the advancement of safe and green industrial synthesis processes and implementing the use of a toolbox system for hazard screening developed within the programme.

Novel research and new collaborations

To achieve this the programme will perform novel research both within traditional fields of science and in collaboration with different disciplines in chemical research, environmental chemistry, inorganic and organic chemistry, enzyme engineering, catalysis, hazard and risk screening and life cycle management.

Cooperation and joint research between academic and industry partners are planned to enable an environment where scientific edge and industry needs guides the development.

The programme is a large and significant research investment and a first step towards the creation of a research and innovation platform for the expansion of green and sustainable chemistry, both in Sweden and internationally.

Tools for the whole life cycle

Mistra SafeChem is designed to follow the process from an industrial or market demand to produce chemicals with specific properties, via prospective hazard screening and safer and greener synthesis processes to life cycle assessment and material management.

The programme will develop both new knowledge and versatile tools, which will enable the expansion of a green chemistry sector and streamline both the process of market introduction and the required testing, registration and reporting according to current legislation.

John Munthe,
IVL Swedish Environmental Research Institute,
Programme director
for Mistra SafeChem.

Richard Lihammar,
IVL Swedish Environmental Research Institute,
Programme manager
for Mistra SafeChem.

With the industry partners involved, the full value chain for chemicals is present, from base chemical producers to users and producers of consumer goods over to those handling of products after use, either as waste or starting material for a circular process.

Collaboration is essential

The programme is constituted of five research work packages, which you can read more about in the coming pages. The collaboration between them will be a key component.

By identifying potential interaction points we hope to create cross-functional studies for testing and application of the tools and processes developed in the programme. In the interactions, we hope to create a better understanding of the requirement and identify possibilities to increase sustainability in the chemical industry in Sweden.

What happened in 2020?

The programme was officially started with the signing of the programme agreement in May 2020. Kick-off for all participants was held in June, digital of course due to the pandemic. Certainly, the pandemic has not been ideal for setting up such a large programme, but despite this work came off with a good start during the autumn.

A management group has been formed, with representatives from all work packages. The group meets once per month and follows up on on-going activities and deliverables as well as plans for the route forward.

The programme board has been established and had its first two meetings. Apart from giving their views and support for the successful management of the programme the board has approved the plans for internal and external communication, procedures for decisions on programme reserve funds and new partners and the programme plan for 2021.

Research started and several scientific articles were published already during the autumn. Internal routines for administration and communication and an external website was created.

During the year the EU's chemicals strategy for sustainability towards a toxic-free environment was published. It stakes out the EU's route towards safer and more sustainable use and production of chemicals. Many of the key elements in the strategy are well aligned with the plan for research within Mistra SafeChem. The strategy, together with the launch of the Horizon Europe program in 2021, also provides an opportunity for Mistra SafeChem partners to engage in international networks and new research collaborations to strengthen and expand the research and innovation on safe and sustainable chemistry in the EU.

With this strategy in hand and the creation of Mistra SafeChem's research and concept of green chemistry in Sweden, we look forward to the coming year with the programme, dedicated to making a lasting change for the chemical industry in Sweden.

SHORT FACTS

This is Mistra SafeChem

Organisation

The research programme is constituted by a consortium of six research partners and twelve industry partners. The consortium, funded by Mistra and the partners, is led by IVL Swedish Environmental Research Institute and report to the Programme Board.

Programme board

Krister Holmberg
Professor Emeritus, Chalmers (Chair)

Patrik Andersson
Professor, Umeå University

Therese Jacobson
Head of Department,
Swedish Society of Nature Conservation

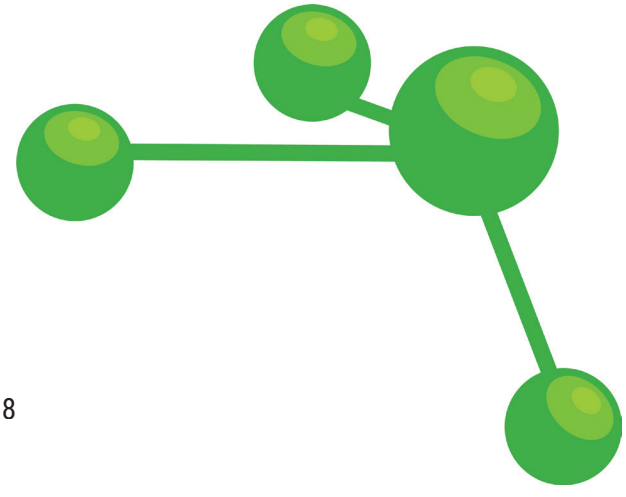
Anna Wiberg
Program Manager, BioInnovation

Per Ängquist
Director General, Swedish Chemicals Agency

Malin Lindgren, co-opted
Programmes Director, Mistra

Research partners

- International Chemical Secretariat (ChemSec)
- Technical University of Denmark (DTU)
- IVL Swedish Environmental Research Institute
- Royal School of Technology (KTH)
  Fibre and Polymer Technology
  SciLifeLab
- RISE Research Institutes of Sweden and RISE IVF AB
- Stockholm University
  Department of Computer and System Sciences
  Department of Environmental Science
  Department of Materials and Environmental Chemistry
  Department of Organic Chemistry



Industry partners

- AC2T Research GmbH
- AstraZeneca
- BASF
- Holmen
- H&M
- IKEM
- Krahnen GmbH
- Perstorp
- RenFuel
- Stockholm Vatten och Avlopp
- Volvo Cars
- Wargön Innovation

Running time

December 2019 – June 2024

Financier and budget

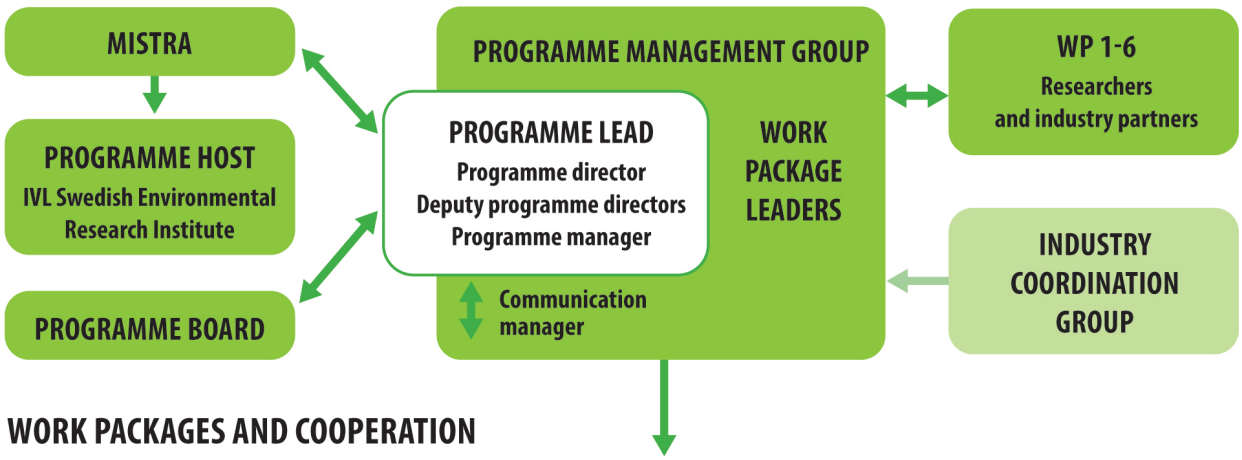
In total 100 MSEK

- 70 MSEK from Mistra
- 4.25 MSEK as cash contribution from industry partners
- 26 MSEK as in-kind contribution from research and industry partners

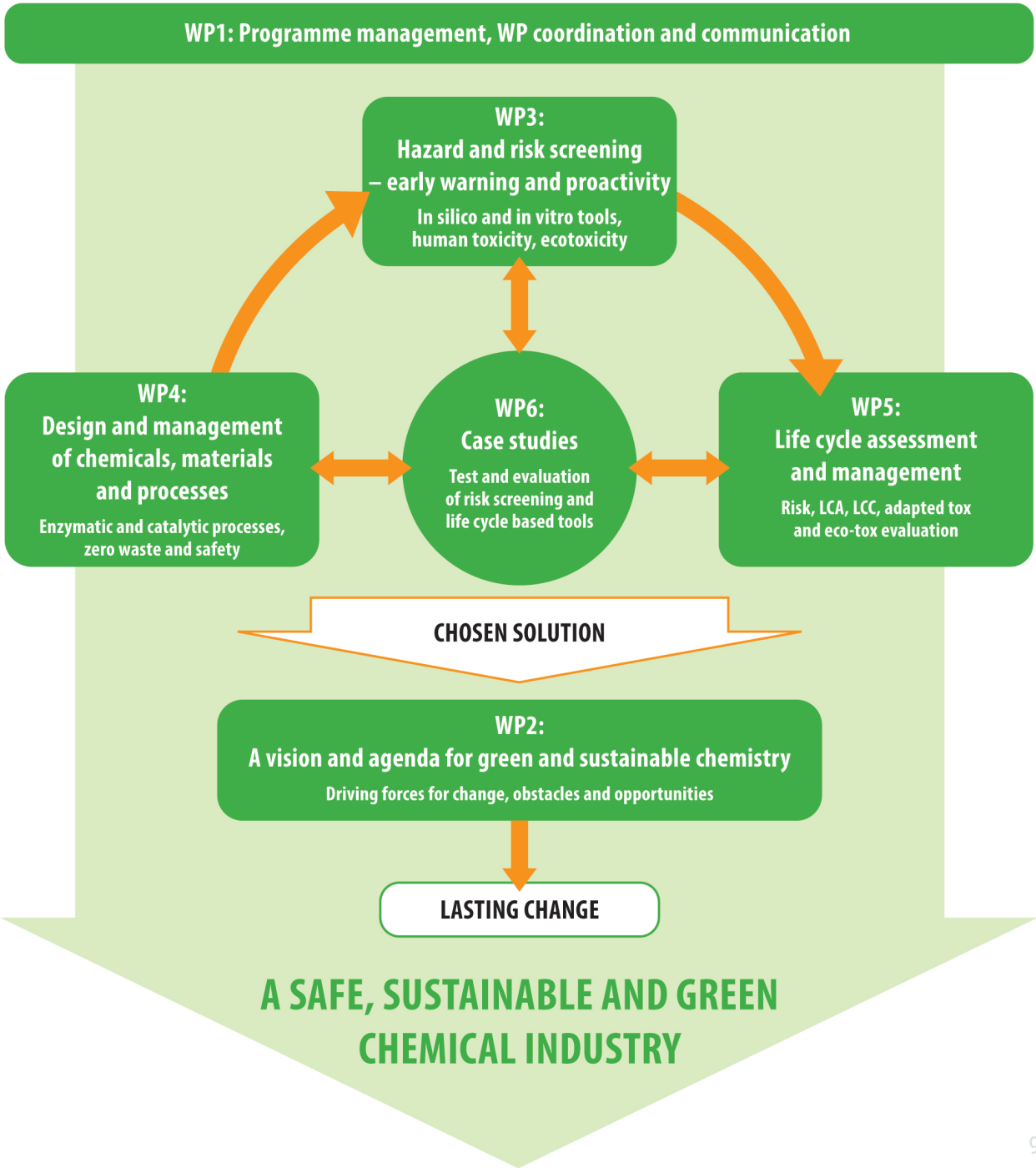
Work packages

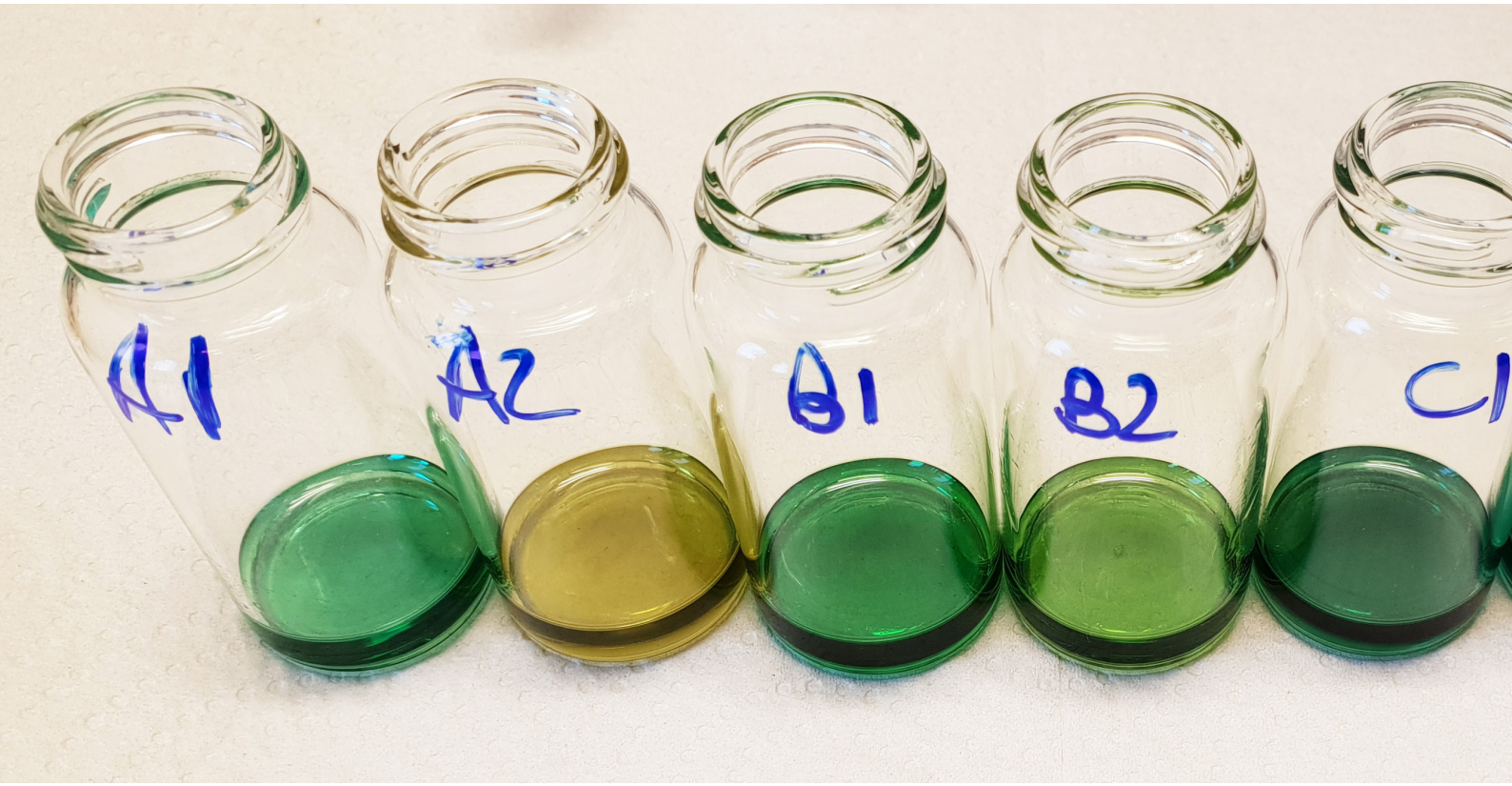
- **WP1:** Programme management, WP coordination and communication
- **WP2:** A vision and agenda for green and sustainable chemistry
- **WP3:** Hazard and risk screening – early warning and proactivity
- **WP4:** Design and management of chemicals, materials and processes
- **WP5:** Life cycle assessment and management
- **WP6:** Case studies

ORGANISATION OF MISTRA SAFECHEM



WORK PACKAGES AND COOPERATION





WORK PACKAGE 2: A VISION AND AGENDA FOR GREEN AND SUSTAINABLE CHEMISTRY

The focus is to integrate the results into an agenda for development

The expertise of our WP

The main focus of WP2 is to integrate the concepts of sustainability and green chemistry with the results of the research in the programme to a vision and a future agenda for development and change. To support this, the WP also complements the main experimental and computational parts of the programme with activities related to sustainable and green chemistry education and regulatory aspects.

The development of the vision and agenda will be made in several steps starting with defining an initial concept followed by an analysis of opportunities and obstacles for the development of a green and sustainable chemistry in Sweden. The concept will be based on information such as types of chemical industry facilities and statistics on import, production, export and use of chemicals.

Results from the research activities in other work packages will be fed into the conceptual framework as they become available and the concept modified in steps.

WP2 also includes the overall programme synthesis where final results from WP3 to WP6 will be integrated and assessed in relation to the conceptual framework.

The participants in WP2 represent IVL, Stockholm University, KTH and RISE. All have long experience in thematic research on chemistry, materials, environment and sustainability as well as from leading and coordinating large research programmes. Industry partners, represented by IKEM, AstraZeneca, Volvo Cars and Perstorp, will provide important input on existing plans and visions as well as their perspective on green and sustainable chemistry.

Extracts of reactions containing colourful compounds and salts, such as porphyrins or chromium complexes.

Achievements in 2020

The first year of the programme was focussed on planning and preparation as well as investigating potential sources of information. Internal engagement of research and industry partners was also initiated.

Purpose of interaction with other WPs

WP2 is dependent on strong interactions and collaboration with all WPs, both in the development of the initial conceptual framework and for integrating and synthesize the results.

All programme partners, research and industry, will also be invited to contribute to the final vision and agenda.

Our goals for the end of the programme

The main goal for WP2 is to present and publish a vision and agenda for sustainable and green chemistry in Sweden. Included in this is to set the path and target for the development of a permanent platform for research, education and implementation of green and sustainable chemistry in Sweden – to be further developed in phase 2 of Mistra SafeChem.

FACTS ABOUT WP2

A vision and agenda for green and sustainable chemistry

Objectives

- To define a conceptual structure for green chemistry in Sweden.
- To assess opportunities and obstacles in markets and policies for expanding green chemistry in Sweden.
- To identify and assess novel evaluation criteria in the legal framework.
- To create a vision and agenda for green chemistry in Sweden.
- To prepare for establishment of a permanent platform for research and implementation of green chemistry.
- Competence development, education and communication.

WP lead

John Munthe, IVL Swedish Environmental Research Institute

Lennart Bergström, Stockholm University

Participants

AstraZeneca, IKEM, IVL Swedish Environmental Research Institute, KTH, Perstorp, RISE IVF, Stockholm University and Volvo Cars.

Activities

- Surveys
- Data gathering and evaluation
- Workshops
- Dialogue

Daphnia (water flea) is used in the "in vitro" toolbox.

WORK PACKAGE 3: HAZARD AND RISK SCREENING – EARLY WARNING AND PROACTIVITY

Three toolboxes for process studies developed in the first year

The expertise of our WP

The core of expertise provides hazard and risk assessments for life cycle analysis of individual case and process studies. Key competencies in computational and AI approaches in toxicology are provided by RISE AB and RISE IVF, ChemSec, AstraZeneca and Stockholm University. These are flanked by competencies within Stockholm University, AstraZeneca and RISE AB in hazard screening in cell-based screening models of human and ecotoxicological toxicities.

The WP also contains key competencies from Stockholm University and IVL Swedish Environmental Research Institute in identification and quantitation of organic chemicals in complex mixtures, using highly sensitive and selective targeted (suspect-driven) and non-targeted chromatographic-mass spectrometric platforms. RISE AB and RISE IVF contain considerable experience in developing risk assessments under a variety of regulatory frameworks in the EU.

Achievements in 2020

During the first year, the WP has developed three toolboxes for application in the individual case and process studies.

The *in silico* toolbox contains about 30 computational tools used to predict a wide variety of human and ecotoxicological hazards, which are relevant to comprehensive early screening and decision steering in the individual case and process developments. The toolbox also contains prediction models for physico-chemical properties, biological degradation and accumulation potential

in the human and ecotoxicologically-relevant species. The tools have been assimilated from public sources and existing sources in partner organisations. New tools utilizing cutting-edge machine learning have also been developed, focussed on endocrine disruption.

The *in vitro* toolbox contains cell assay systems capturing one or several aspects of hazards related to chemical exposures. The systems complement *in silico* predictive models by capturing toxicity potential in a variety of cell systems representing human organ/tissue toxicities relevant to the case and process studies (e.g. liver, skin, immune system, lung, endocrine tissue) and ecotoxicological signal species such as Daphnia and microalgae. The toolbox also includes a high-throughput screening platform using advanced high content imaging techniques and robotic-controlled combinatorial exposures.

The analytical toolbox involves targeted and non-targeted analytical techniques to cover non-volatile and semi-volatile compounds in complex mixtures. This also includes computational tools for structure designation of new emerging unknowns and coupling these to hazard prediction tools.

Purpose of interaction with other WPs

Liaison persons have been assigned to each case study in WP6 and process themes in WP4. These are delineating plans for the fit-for-purpose application of *in silico*, *in vitro* and analytical approaches in each of the studies. The purpose is to provide iterative guidance on changes to basic chemistries/material compositions and process chemistries which should be pursued in seeking more green and sustainable alternatives.

To fully assess the consequences of chemistry/process changes, the data generated in WP3 will be fed into appropriate life cycle based assessments conducted by WP5. Liaison between WP3 and WP5 will be further enhanced by the initiation of a PhD student who will work on digitalisation methods for channelling *in silico* and *in vitro* hazard data into the various life cycle based assessment tools used.

Our goals for the end of the programme

To provide a sustainable platform of fit-for-purpose tools for hazards and exposure screening and assessment, and well-defined routes of application, supporting changes to chemistries and processes yielding green and sustainable industrial processes and materials that are “safe by design”.

FACTS ABOUT WP3

Hazard and risk screening – early warning and proactivity

Objectives

WP 3 will construct and maintain a framework of capabilities and competencies providing a workflow moving through the following steps:

- Initial mitigation planning for hazard identification, exposure estimations and risk assessment, from both the human and environmental perspectives.
- In silico screening of available human and ecotoxicological/environmental fate data, read-across data by structural QSAR and application of other predictive computational toxicological tools.
- In vitro screening for critical human and ecotoxicological adversities relevant for risk assessment, including for combinatorial exposures.
- Development and application of analytical methodologies and techniques, including non-target analyses of exposures and bio-stability, particularly from the ecosystem perspective.
- Integrated hazard and risk assessments which are fit for purpose in appropriate material/process developments and case studies.

WP lead

Ian A Cotgreave, RISE AB

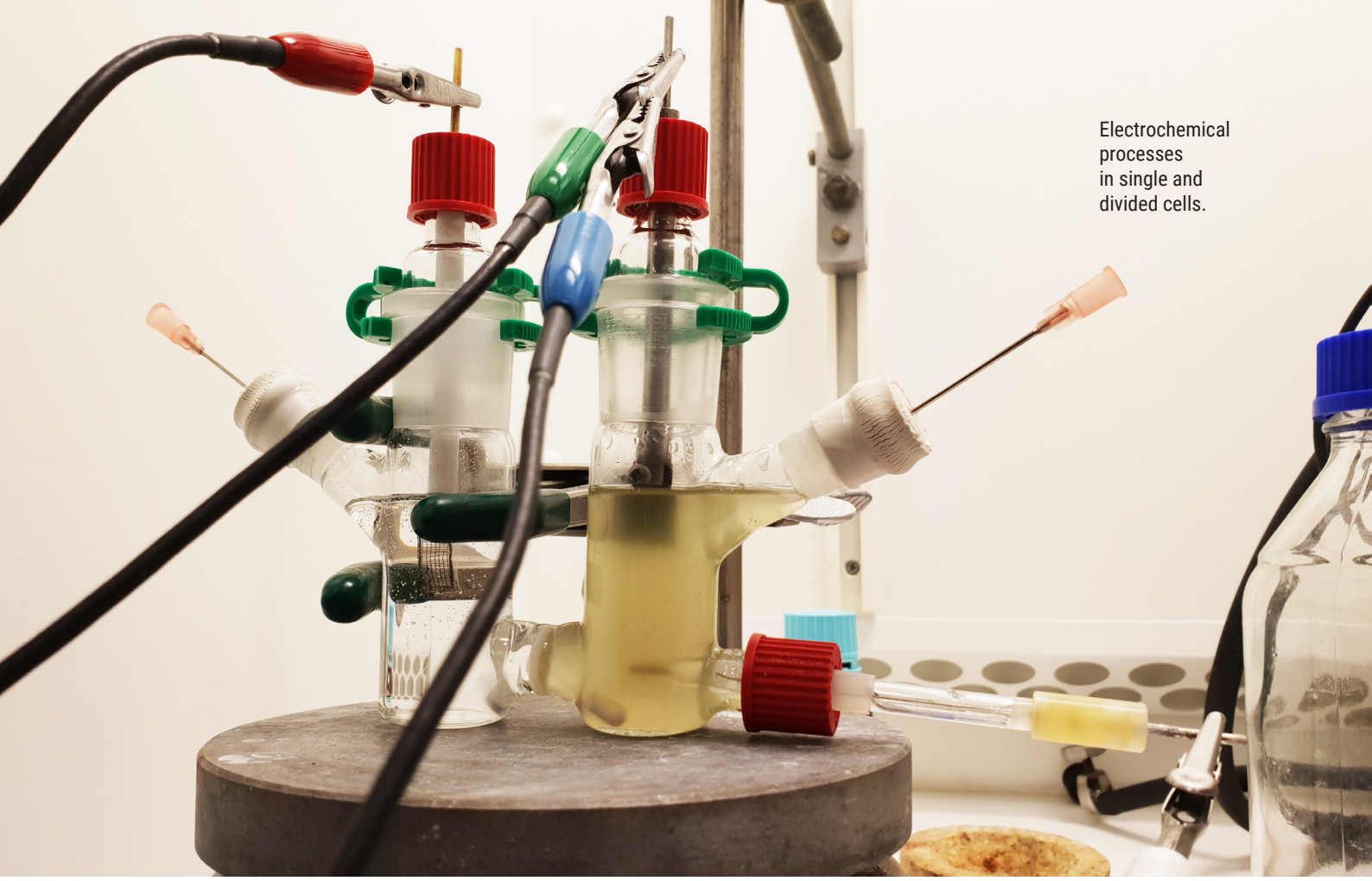
Magnus Breitholtz, Stockholm University, Environmental Science

Participants

AstraZeneca, ChemSec, IVL Swedish Environmental Research Institute, RISE AB, RISE IVF, Stockholm University (Computer and Systems Sciences, Environmental Science, Materials and Environmental Chemistry, and three new PhDs).

Activities

- Computational toolbox established for hazard screening.
- New computational tools developed in the area of endocrine disruption hazard prediction.
- Key PhD positions filled.
- Key inter-WP liaisons and working routines established.
- Initial risk mitigation planning performed with the industrial cases.
- Computational hazard data delivered to one of the industrial cases.



Electrochemical processes in single and divided cells.

A close collaboration to provide green methods and materials

The expertise of our WP

The aim of WP4 is to develop synthetic procedures to access the production of chemicals and materials within the principles of sustainable chemistry by developing atom- and energy-efficient routes using catalysts of different nature, and by generating new knowledge and tools.

WP4 is working closely with the industry to incorporate new sustainable methods into its existing platforms. Participants include experts and leading scientists in several areas related to green and sustainable processes for new chemicals and materials. Specific areas of expertise include:

• Materials and methods for energy and environmental applications using electrochemistry, solid-state chemistry, photocatalysis, ssNMR spectroscopy, bio-inorganic composites and TEM.

• Processing of biobased materials and use of nanoscale cellulose as a building block enabling development of biobased adsorption membranes, biomedical implants, spun fibres, antifouling and antibacterial coatings.

• Transformations of biomass, in particular development of routes to valorize technical lignin.

• Enzyme- and transition metal-catalyzed organic reactions including heterogeneous transition metal catalysts for the synthesis of complex organic compounds, fine chemicals and pharmaceuticals.

• Chemoenzymatic catalysis and enzyme design and engineering for expedient green chemical synthesis. New methodological frameworks for accelerated biocatalysis with an emphasis on amide bond synthesis for polymer and pharmaceutical applications.

• Development of new efficient catalytic procedures for the construction of carbon-carbon and carbon-heteroatom bonds including design of new and novel catalysts. Combining experimental and theoretical tools to understand structure-activity relationships.

Achievements in 2020

The achievements include the development of an advanced nanoscale spectroscopic TEM EELS & EDX method for analyzing complex compositions and the development of an N-doped carbon catalyst for electrochemical denitrification.

In the area of catalytic fractionation, a methodology directed towards forestry residues has been developed. For textiles, the team has developed a method to separate synthetic polymers from cellulose and depolymerization of plastics.

Within the area of catalysis, we have developed several selective oxidative cascade reactions where palladium was immobilized. We have also developed a new method to generate stable and active enzymes.

Another achievement is a robust, carboxylate-directed C-H methylation of benzoic acids with applications to clinically used drugs. The team has reported a solvent recycling system. The methodology was also expanded to d3-methylation, granting rapid access to the isotope-labelled drugs.

Purpose of interaction with other WPs

WP4 has initiated studies on toxicological assessment of particle-based hazards with WP3, as well as ecotoxicology studies on chemicals generated during benign transformations of biomass and regeneration of textiles. The toxicity of the chemicals and products involved in the different processes developed will be also studied in collaboration with WP3. Life-cycle based assessment of selected processes will be done in cooperation with WP5.

Our goals for the end of the programme

Overall WP4 aims to contribute towards green chemical manufacturing. By the end of the programme, we expect to be able to minimize nanoparticle-based hazards and replace metal particles in several applications by providing green methods or materials, develop value chains from forestry residues and also textiles to streams of valuable platform chemicals and materials, and to substitute metal catalysts based on precious metals by catalysts constructed from abundant and non-toxic metals.

We also expect Mistra SafeChem to contribute to implementing green chemistry into our students' intended learning in the bachelor, master and PhD programs.

FACTS ABOUT WP4

Design and management of chemicals, materials and processes

Objectives

- Optimize material use, re-use and recycling for maximum benefits for resource efficiency and sustainability.
- Develop green chemistry industrial processes aiming at replacing/minimizing the use of toxic chemicals and minimizing waste.
- Rational design of first-row transition metal and enzyme catalysts,upscaling of green catalytic processes towards industrial scale.
- Development of methods to define and quantify resource efficiency and circularity of value chains.
- Providing data for evaluation and understanding toxicology determinants of the developedprocesses

WP lead

Belén Martin-Matute, Stockholm University
Per-Olof Syrén, KTH

Participants

AC2T Research, AstraZeneca, Holmen, Krahnen, KTH, Perstorp, RenFuel, Stockholm University, Wargön Innovation. Six PhD students and four PostDocs.

Activities

- Major progression to convert tops and branches to dissolving grade quality
- Major progression to isolate cellulose nanocrystals from dyed and undyed cotton
- Initial progression in depolymerization of polyesters in textiles
- Initial progression in isolating cellulose and polymers (PET or acrylics) from textile blends
- Developed a method to generate stable and active enzymes for industrial applications
- Significant progress made in biocatalytic amide bond formation
- Developed an electrochemical method for the reduction of unsaturated compounds base on non-precious chemicals
- Developed of an advanced nanoscale spectroscopic TEM EELS&EDX method for analyzing complex nanoparticle compositions
- Developed an N-doped carbon catalyst for electrochemical
- Cross-collaborative work started with industrial partners
- Established work routine and agreement on cases for non-targetted screening (WP3) and LCA (WP5)

A paper on chemicals of concern in plastic toys is one of many important contributions to the Mistra SafeChem toolbox development.

WORK PACKAGE 5: LIFE CYCLE ASSESSMENT AND MANAGEMENT

The main goal is to develop a life cycle based assessment toolbox

The expertise of our WP

WP5, Life cycle assessment and management, gathers researchers from the two Swedish research institutes IVL Swedish Environmental Research Institute and RISE IVF, and the Technical University of Denmark (DTU).

This group of researchers have vast experience in life cycle based assessments generally, and life cycle assessment (LCA) and life cycle impact assessment (LCIA) specifically. We are at the forefront of advancing tools and methods for the characterization of ecotoxicological and toxicological effects in life cycle based assessments.

Engaged in the work package (WP) are also industrial partners from BASF, AstraZeneca, Volvo Cars and Perstorp, providing important perspectives from their respective fields and making industry based real-life case studies possible.

Achievements in 2020

In 2020 effort was placed in coordination, within the WP and with other WPs in the programme, and in the work on further detailing tasks within the WP, including plans for defining a jointly supervised PhD project in support of increased collaboration of WP5 with the other programme WPs.

As one of the main tasks is the development of a toolbox for life cycle based assessments, a key achievement was that researchers and industrial partners joined forces and wrote an abstract that was accepted as a platform presentation at the Society of Environmental Toxicology and Chemistry (SETAC) Europe 2021 conference: “A life cycle

based assessment toolbox to assess and improve safety and sustainability of chemicals". Key for the toolbox development is a number of case studies, in which the available and newly developed tools and data can be tested, and additional research and data development needs are identified.

In 2020 work was started in the case studies connected to WP6 and additional case studies were planned. Furthermore, DTU and colleagues had two papers accepted for publication in scientific journals, one on a tiered framework for quantitatively assessing exposure and life cycle impacts in chemical alternatives assessment (CAA) and another on chemicals of concern in plastic toys, both important contributions to the programme's toolbox development.

Purpose of interaction with other WPs

WP5 interacts with WP3, 4 and 6 by joint model and data development, case studies and trainings. These interactions make it possible to create a toolbox for life cycle based assessment that is well suited for the aims of the programme as a whole, with case studies capturing different challenges with relevance for the expansion of sustainable chemical industry and a toxic-free environment.

By direct collaboration with WP3 aims are to advance data generation and application by digitalization. Trainings dedicated to WP4 research groups aim to equip the researchers to make sustainability assessment but also to identify interesting cases for further study.

Our goals for the end of the programme

The main goal of WP5 is to develop a life cycle based assessment toolbox, with an associated guideline, to assess and improve the safety and sustainability of chemicals. The toolbox is foreseen to be applied to CAA in substitution as well as process development and optimization.

The methods and tools in the toolbox are on the one hand compliant with the conditions of rapid-screening assessments in CAA and using comparative metrics in both CAA and LCA, and on the other hand they are overcoming the limitations of currently applied data and methods.

The goals are furthermore to execute several case studies and to collate data generated in case studies in a dedicated database. With focused trainings for the programme partners in other WPs, they will be able to apply the toolbox in additional case studies.

FACTS ABOUT WP5

Life cycle assessment and management

Objectives

- To develop and provide a life cycle based toolbox for high throughput alternatives assessment for chemical substitution.
- To develop a model fit-for-purpose for estimating near-field human exposure for different product application contexts for integration into life cycle assessment and alternatives assessment.
- To provide ProScale/ProScaleE and USEtox LCIA characterization factors for human toxicity and eco-toxicity for all case study relevant chemicals that are within the scope of the included methods.
- To build a database compiling all relevant information from LCA carried out from case studies.
- To deliver guidelines and training on how to apply life cycle approaches/assessment in case studies and along the design process.

WP leads

Hanna Holmquist,
IVL Swedish Environmental Research Institute
Anna-Karin Hellström, RISE IVF

Participants

AstraZeneca, BASF, DTU (including one PhD student) IVL, Perstorp, RISE IVF, Volvo Cars,

Activities

- Inter/intra WP coordination
- Initiation of case studies
- Scoping of the life cycle based toolbox
- Advancement of models within the toolbox

Two case studies started in 2020: one on cosmetics, the other on air quality and materials inside cars.

WORK PACKAGE 6: CASE STUDIES

In the case studies the ideas are put into practise

The expertise of our WP

The focus in WP6 is to identify industrial challenges related to green chemistry and translate them into case studies that allow the Mistra SafeChem programme to test and develop its toolbox.

The WP has started two large case studies, one on air quality and materials inside cars and one focussed on finding alternatives to cyclosiloxanes and silicones in personal care products.

New case studies will be set up during the programme. These can be initiated in two ways:

1) Researchers and partners in the project that want to build a case study to develop and test their work

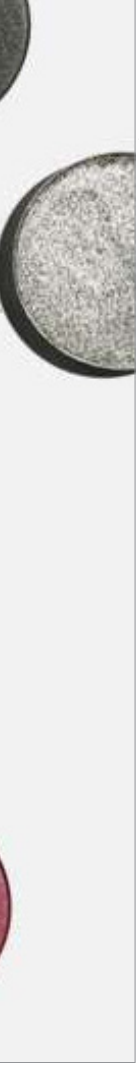
2) Companies that need help with a specific issue, which requires the toolbox developed by Mistra SafeChem

WP6 helps develop and manage these case studies to make sure all partners benefit.

Achievements in 2020

In 2020, WP6 has successfully started the two initial case studies together with Volvo Cars and H&M. A work plan was developed for each case study and a core team with representatives from other WPs has been established.

In the case study for Volvo Cars, different tracks have been developed, depending on the source of information on the presence of hazardous chemicals in the car cabin. These could be results from previous analyses, data from new measurements or questions from suppliers willing to substitute an unwanted chemical with a safer alternative. These tracks will be run in parallel. 2020 ended with a first discussion on how a sampling campaign could be developed and which compounds should



be prioritized for an initial assessment in which the toolbox will be tested. This initial assessment will help coordinate the workflow before the toolbox is used on larger groups of chemicals.

In the case study for H&M, a mapping of type of silicones and amounts used in the H&M product portfolio has been performed, together with a literature search regarding different types of silicones used in cosmetics, their function, production process and environmental fate etc. Also, a toxicology evaluation of commonly used silicones has started using the toxicology toolbox in WP3. All information collected will be used as a ground for selecting which silicones and products to focus on further in the project in terms of alternatives assessment.

Purpose of interaction with other WPs

WP6 helps the other work packages to develop their ideas and research into case studies where they can put those ideas into practise. Here WP6 plays a coordinating role by streamlining the process on how the work packages can be managed.

The case studies foster strong collaboration between the work packages. Representatives from all of them are included in the case studies from the start. They employ the toolbox in the case studies, help keep WP6 updated with news on developments and project ideas from the other work packages and with finding the right expert for the tasks outlined in the case studies. They also keep the other work packages informed on the progress in the case studies, the need for specific help and potential research opportunities within the case studies.

Our goals for the end of the programme

By the end of the programme, WP6 will have expanded its portfolio to include more case studies and new partners into Mistra SafeChem. The experience gained from developing and managing these studies will translate into a format that can easily be applied in a future permanent green chemistry research platform.

The results from these case studies will feedback to the other work packages and help improve the toolbox and address knowledge gaps. It will also help match research initiatives with industry needs.

Through the case studies, WP6 will also contribute to the publication of peer-reviewed scientific research.

FACTS ABOUT WP6

Case studies

Objectives

- To coordinate the interaction between the case studies and the various tools and methods generated in WP3, WP4 and WP5.
- To transform industrial challenges into cases fit for the programme and evaluation of the tools.
- To formulate the results from the case studies into general conclusions with respect to efficiency and reliability of the toolbox.

WP lead

Dämien Bolinius,
IVL Swedish Environmental Research Institute
Lisa Skedung, RISE

Participants

AstraZeneca, H&M, IVL Swedish Environmental Research Institute, KTH, Perstorp, RISE, Stockholm University, Volvo Cars

Activities

- Identification of industrial challenges and translation of those challenges into case studies for Mistra SafeChem.
- Case study 1: Indoor air quality – materials inside the car that do not cause health effects. In collaboration with Volvo Cars.
- Case study 2: Cyclosiloxanes and silicones. In collaboration with H&M.
- Case studies on: Process optimization and intensification.
- Case study summary.

We asked a few of the Mistra SafeChem industry partners why they decided to join the programme.

MISTRA SAFECHEM INDUSTRY PARTNER

Perstorp

Perstorp has the ambition to become a finite material neutral company. We think the Mistra SafeChem programme can enable the way forward and speed up the process.

We manufacture speciality chemicals molecules that end up in a variety of applications, everything from polymers to animal nutrition. All of them have an impact on the environment, for example through the manufacturing process or carbon dioxide emissions. Mistra SafeChem allows us to understand various environmental implications before new intended chemicals have become products. Hence, the company can make early decisions to develop sustainable products and chemicals and reduce risks of investing money and resources in potentially bad projects.

In addition to our sustainable ambition, we hope the close collaboration within the project can help us understand how the other companies relate to the problem and help each other taking the step forward. We think Mistra SafeChem will make it easier to address the product and process development issue through the focused collaboration in the project.

Oleg Pajalic
Principal Scientist, Perstorp

MISTRA SAFECHEM INDUSTRY PARTNER

BASF

We at BASF are committed to continuously minimizing the negative effects of our products on the environment, health and safety – from development to disposal. This commitment to product stewardship is enshrined in our Responsible Care® charter and the initiatives of the International Council of Chemical Associations. We also ensure uniformly high standards for product stewardship worldwide.

We train and support our customers in fulfilling their industry or application-specific product requirements. Together with other manufacturers, BASF is pushing for the establishment of voluntary global commitments to prevent the misuse of chemicals. We are working together with the European Chemicals Agency on a project to improve the quality of REACH dossiers.

In this context, we develop methods for human toxicity and eco-toxicity assessments in LCA as well. We were a partner in the development of the ProScale method and are looking forward to putting this expertise into the Mistra SafeChem programme, to discuss it with other partners and identify how the method in conjunction with others can be further developed and used.

Prof. Dr. Peter Saling,
Director Sustainability Methods,
BASF

MISTRA SAFECHEM INDUSTRY PARTNER

Volvo Cars

Sustainability is central to Volvo Cars' purpose and as important as safety. We aim for the highest standards in sustainability within our industry. We recognize that becoming a truly sustainable business and producing sustainable products is essential for our future success. By taking part in the Mistra SafeChem project we further aim to achieve this goal by addressing the important issues of green chemistry and sustainable substance use in our products. This is also in line with our aim to be a circular business by 2040.

We hope that the programme will further help us address the important issues of substance use in our products and help us make conscious choices when it comes to assessing substances and also addressing the importance of evaluation of the impact of the effects of substances used.

Volvo Cars has a case study within the programme focusing on the interior air and materials to further increase the knowledge about toxicology and life cycle alternative assessments.

Volvo Cars also sees the program as a possibility to interact with other industrial partners in the broad consortium of Mistra SafeChem and see how they address these issues.

Maria Bernander,
Technical Expert, Occupant Health
Effects, Volvo Cars

MISTRA SAFECHEM INDUSTRY PARTNER

AstraZeneca

We think Mistra SafeChem has an important role in educating a new generation of scientists about sustainability and green chemistry. In the interaction between academia and industry, it is important to work together, mix expertise ranging from very theoretical to applied science. By doing so Mistra SafeChem can be a paradigm shift for the Swedish chemical industry and academic research.

LCA and green chemistry principles along with the UN sustainability goals are important but do not offer good measurables. I hope that the programme will add to these overarching goals – to give better instruments for both industry and academia in pursuit of sustainable chemical science, development and production.

The fact that different industries get to work together makes this a unique platform for collaborations. I am confident that we will transform the chemical industry long-term by applying things like improved LCA analyses, better predictive tools for eco/toxicology, improved processes using either chemo or biocatalysis and by educating our staff both in academia as well as industry on these matters.

Magnus Johansson
Associate Professor
and Principal Scientist,
AstraZeneca

PARTICIPANTS IN THE PROGRAMME

Research partners

WP and task leaders from each organisation

- **International Chemical Secretariat (ChemSec)**
  Jerker Ligthart – WP3
- **Technical University of Denmark (DTU)**
  Peter Fantke – WP5
- **IVL Swedish Environmental Research Institute**
  John Munthe – WP1 and WP2
  Richard Lihammar – WP1 and WP2
  Dämien Johann Bolinius – WP6
  Hanna Holmquist – WP5
  Tomas Rydberg – WP5
  Gunnar Thorsén – WP3
- **Royal School of Technology (KTH)**
  Ulrika Edlund, Fibre and Polymer Technology – WP2
  Per-Olof Syrén, SciLifeLab – WP4
- **RISE Research Institutes of Sweden and RISE IVF AB**
  Ian Cotgreave – WP3
  Anna-Karin Hellström – WP5
  Lisa Skedung – WP6
- **Stockholm University**

Department of Computer and System Sciences
Ulf Norinder – WP3

Department of Environmental Science
Magnus Breitholtz – WP3
Oskar Karlsson – WP3
Jonathan Martin – WP3

Department of Materials and Environmental Chemistry
Lennart Bergström – WP1 and WP2
Aji Mathew – WP4
Ulrika Nilsson – WP3
Adam Slabon – WP4

Department of Organic Chemistry
Jan-Erling Bäckvall – WP4
Belén Martín-Matute – WP4
Joseph Samec – WP4

Industry partners

Contact persons at each organisation

- **AC2T Research GmbH** – Serhiy Budnyk
- **AstraZeneca** – Magnus J Johansson
- **BASF** – Peter Saling
- **Holmen** – Jörg Brücher
- **H&M** – Haiyan Chen Gallstedt
- **IKEM** – Nils Hannerz and Kristina Neimert Carne
- **Krahnen GmbH** – Pascal Lohmann
- **Perstorp** – Oleg Pajalic
- **RenFuel** – Clara Pierrou
- **Stockholm Vatten och Avlopp** – Katja Närhi
- **Volvo Cars** – Maria Bernander
- **Wargön Innovation** – Joel Arnoldsson

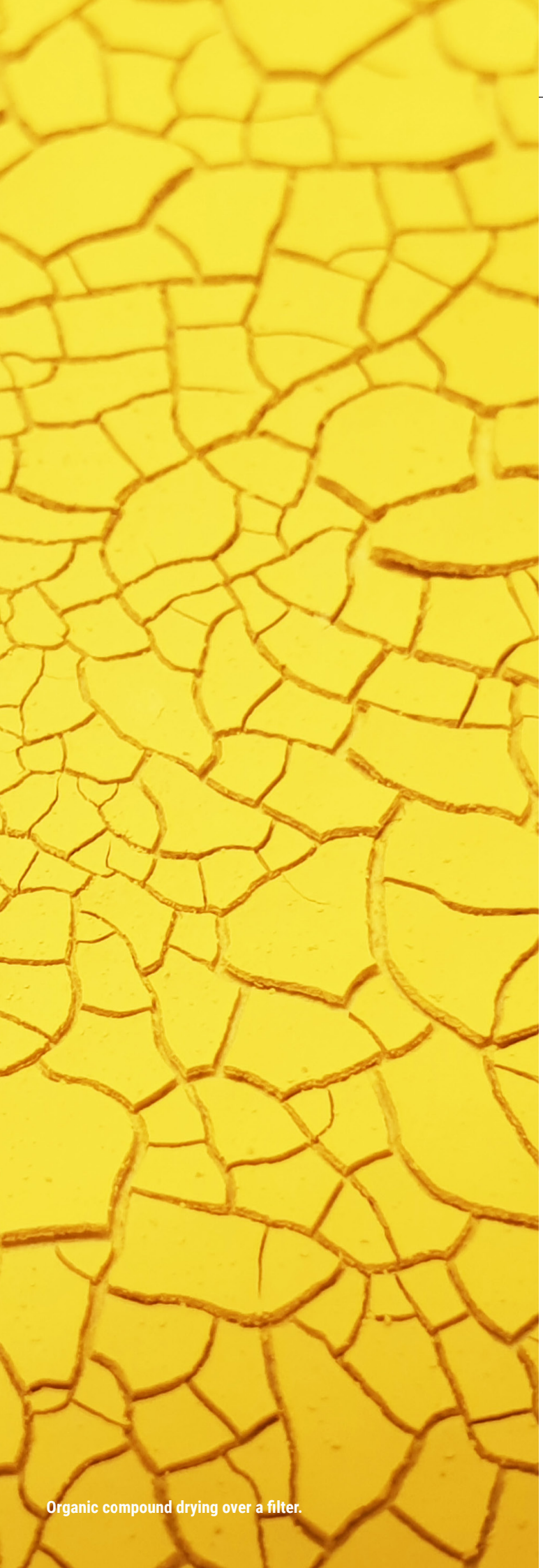
DELIVERABLES 2020

Administrative

- Programme plan year 1
- Programme website: mistrasafechem.se
- Consortium agreement
- Kick-off meeting with all partners June 17, 2020
- Communication plan year 1
- Programme plan year 2

Scientific publications

- M-B Li, Y Yang, A A Rafi, M Oschmann, E Svensson Grape, A K Inge, A Córdova, J-E Bäckvall (2020) Silver-Triggered Activity of a Heterogeneous Palladium Catalyst in Oxidative Carbonylation Reactions. Angewandte Chemie 9, 10391
- T M Budnyak, A Slabon, M H Sipponen (2020) Lignin–Inorganic Interfaces: Chemistry and Applications from Adsorbents to Catalysts and Energy Storage Materials. ChemSusChem 13, 4344
- P Fantke, L H, M Overcash, O Jolliet (2020) Life cycle based alternatives assessment (LCAA) for chemical substitution. Green Chemistry 22, 6008
- I Szewczyk, A Rokicińska, M Michalik, J Chen, A Jaworski, R Aleksis, A J Pell, N Hedin, A Slabon, P Kuśtrowski (2020) Electrochemical Denitrification and Oxidative Dehydrogenation of Ethylbenzene over N-doped Mesoporous Carbon: Atomic Level Understanding of Catalytic Activity by 15N NMR Spectroscopy. Chemistry of Materials 32, 7263
- J Onwumere, J Piątek, T Budnyak, J Chen, S Budnyk, Z Karim, T Thersleff, P Kuśtrowski, A P Mathew, A Slabon (2020) CelluPhot: Hybrid Cellulose–Bismuth Oxybromide Membrane for Pollutant Removal. ACS Applied Materials and Interfaces 12, 42891
- T Thersleff, S Budnyk, L Drangai, A Slabon (2020) Dissecting complex nanoparticle heterostructures via multimodal data fusion with aberration-corrected STEM spectroscopy. Ultramicroscopy 219. 113116



Organic compound drying over a filter.

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Management group/WP-leaders

WP1 leaders

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Richard Lihammar, IVL

WP2 leaders

John Munthe, IVL Swedish Environmental Research Institute
Lennart Bergström, Stockholm University

WP3 leaders

Ian Cotgreave, RISE
Magnus Breitholtz, Stockholm University

WP4 leaders

Belen Martín-Matute, Stockholm University
Per-Olof Syrén, KTH

WP5 leaders

Hanna Holmquist,
IVL Swedish Environmental Research Institute
Anna-Karin Hellström, RISE IVF

WP6 leaders

Dämien Johann Bolinius,
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Website

mistrasafechem.se

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