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# UPDATE CATALISTI INNOVATION AGENDA

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# Introduction

With this document, Catalisti proposes an update of its Innovation Agenda. The Innovation Agenda is the concretisation of Catalisti's ambition to achieve a sustainable and competitive chemicals and plastics converting industry in Flanders by an innovative power of world class. This Innovation Agenda forms the guideline for all Catalisti activities, not in the least for the initiation and evaluation of its innovation projects.

This update is drafted by the Catalisti team based on different resources and contributions. Alignment with individual company roadmaps and with the research agendas of our knowledge partners was ensured by organising a feedback round and a discussion with the members of the Industrial Advisory Board. Several international innovation agendas and roadmaps were used as benchmark and inspiration. Multiple references to the SusChem SIRA can be found throughout the document.

Major novelties that have been introduced in this 2020 version are:

- a new name for all four Innovation Programs, better reflecting the content of each program;
- an explicit description of the goals of each program and the way projects should contribute to these goals;
- an elaboration of the content of each program based on a list of concrete topics described in more detail.

The four newly named Innovation Programs are: 'Biobased Value Chains (BVC)', 'Process Intensification and Transformation (PIT)', 'Circularity and Resource Efficiency (CRE)', and 'Advanced Sustainable Products (ASP)'. Although each program has its own content and goals, there are significant interfaces between the programs. In addition, there are also different links with the Moonshot Research Trajectories (MOTs) of the Flanders Industry Innovation Moonshot. Both the interfaces between the Catalisti programs as well as the links between the Catalisti programs and the MOTs are described.

The list of topics within each Innovation Program gives a good indication of the content of the program but is not limitative. This means that project ideas that fall outside the listed topics can also be considered if they have the potential to contribute to the goals of the program. The stage of development of the different topics within Catalisti is diverse: for some, an extensive project portfolio with important results has already been achieved, for others, first activities must still start.

The overarching objective of delivering sustainable innovation is safeguarded by performing a sustainability assessment at different stages of project development, execution and evaluation. In order to do so, Catalisti has developed a "Sustainability Assessment Tool" or SAT in collaboration with its members and external experts. The SAT is a "life cycle thinking"-based, simple and accessible instrument in which major environmental impacts over the different phases of the life cycle are mapped and analysed. It is based on the input of qualitative data, which can be complemented over the course of a project by quantitative data.

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# Biobased Value Chains (BVC)

## What

In this innovation program, we use biobased resources as feedstock to develop and produce biobased chemical products. All types of biobased resources can be used, including primary biomass coming from agriculture or forestry like sugar beets, plant-based oils and wood, new biomass sources like insects or algae, and secondary biomass like organic waste and agricultural or industrial by-products.

For the conversion of such biobased resources to chemical products, different technologies can be used. In this innovation program, we focus on chemical catalysis, enzymatic catalysis and fermentation as the more established processes to convert biobased resources, while other technologies are listed in ‘Process Intensification and Transformation’. These conversion technologies are used in combination with upstream and downstream technologies like extraction, separation and/or polymerisation.

Biobased chemicals can be platform molecules that have the potential to become the core of new biobased value chains, but also specialty chemicals that are developed from an application perspective. While developing biobased chemicals, we focus on the functionality they can bring in their application. We do not specifically focus on biodegradability, although this can be a beneficial functionality for some products in some applications.

## Why

The two most important drivers for the development of biobased value chains are the potential for feedstock diversification and the potential for new functionalities when designing biobased products. As the structure and composition of biobased resources is completely different from that of fossil resources, the use of biomass brings a whole palette of possibilities to develop new building blocks and new functionalities. This also brings the opportunity to acquire interesting intellectual property positions.

In addition, the use of biobased resources as feedstock for chemical products has the potential to reduce the overall environmental impact of chemical value chains. When comparing $CO_2$ emissions over the life cycle of biobased products with their fossil-based counterparts, biobased products have the advantage of a negative contribution in the growth phase of the biomass, as the carbon was captured through photosynthesis in the biomass. Also, specific processes used to convert biomass like enzymatic catalysis and fermentation have the potential to significantly reduce the $CO_2$ emissions of the production process.

## Goals

The goal of the Biobased Value Chains program is to develop a number of ‘new’ biobased value chains each year, from feedstock over conversion process up to product in the market. A ‘new’ value chain is based on an innovation in at least one of the three phases of a biobased value chain, while safeguarding the valorisation potential of the whole value chain.

By doing so, we want to prove that biobased chemicals can indeed:
- contribute to decreasing the chemical industry’s dependency of on fossil resources;
- deliver new functionalities in existing or new applications;
- connect non-traditional players;
- help to decrease the overall environmental impact of chemical value chains;
- help our member companies to acquire interesting IP positions.

# Topics

## Lignocellulose

### *What*

Lignocellulosic biomass (i.e. non-edible biomass such as wood, straw, corn stover, agricultural or forestry residues and grasses) is composed of three polymer constituents, being lignin, cellulose and hemicellulose. The ratios of the different constituents can vary significantly depending on the biomass source.

Lignin is a complex polymer of phenolic type moieties and can be considered the most abundant source of renewable aromatics on earth. It is therefore generally regarded as a promising – yet challenging – future feedstock towards sustainable biobased aromatics.

Cellulose and hemicellulose, on the other hand, are both polysaccharides. While cellulose is a linear polymer consisting of only D-glucose units, hemicellulose has a branched structure consisting of different sugar molecules. Besides glucose, these sugar molecules can for instance be C5 sugars like xylose and arabinose and C6 sugars like mannose and galactose.

To start exploiting these polymers, the biomass needs to be broken down into its constituents in a biorefinery. The most well-known example of such a biorefinery is a paper mill, where (hemi)cellulose fibres are used to make paper products. Due to the harsh conditions applied in paper mills, the resulting lignin is more condensed (than its natural form) and more difficult to further process (depolymerise) into chemical building blocks. Until recently, it was therefore considered a waste product and burned for its energetic value. Nowadays, different actions are taken to create more value out of this ‘waste’ lignin, for instance by (partial) depolymerisation.

In another and more recent ‘lignin-first’ biorefinery approach, separation of the constituents is combined with depolymerisation of the lignin fraction in one process, retaining as much functionality of the lignin fraction as possible. This results in a lignin oil composed of lignin monomers, dimers and oligomers, leaving behind the (hemi)cellulose fraction as a side product. This (hemi)cellulose fraction can then, for example, be used as a carbohydrate feedstock for fermentative processes (after further processing and depolymerisation), but also for all kinds of composite materials in its polymer fibre form.

### *Why*

The biggest driver of the use of lignocellulosic biomass is its abundance and local availability, and as such a replacement of fossil resources. In the specific case of lignin, the functionality inherently present in the resulting phenolic monomers and oligomers is a second important driver for the use of lignocellulose as a feedstock.

### *State-of-play*

Since the start of Catalisti (FISCH), lignocellulose as a feedstock has played an important role in the biobased innovation program. Starting with low-TRL projects like ARBOREF and MAIA focusing on the lignin-first approach, a proof of concept has been shown for a number of different applications. More recently, the depolymerisation/functionalisation of lignin side streams is also been investigated in the BIORESAL project. In parallel, a lot of effort has been invested in mapping of the state-of-the-art of the different technologies and feedstocks in the BAFTA project, leading to a comprehensive overview. And finally, different initiatives are running (e.g. LignoValuePilot @VITO, BIOCON @KU Leuven, Moonshot PILLAR project) into upscaling of selected technologies to provide industry with larger samples to assess the feasibility on a relevant industrial scale. This has been a severe bottleneck in most of the projects until now. These examples are complemented by several other funded projects (EU, FWO, etc.) regarding this topic.

### *Next steps*

All these actions should ultimately reduce the risk to invest in a future lignocellulose processing demonstration plant in Flanders. Together with the development of new applications to broaden the added value, this should then lead to the establishment of a full lignocellulose value chain.

## Sugars

### *What*

Sugars, or carbohydrates, are a broad set of different compounds divided into four chemical groups, i.e. mono-, di-, oligo- and polysaccharides. Within these four groups, further distinction can be made in terms of regio- and stereoselectivity, but also regarding the presence of heteroatoms besides carbon, hydrogen and oxygen.

This topic therefore covers the use of the following feedstocks:

- first generation feedstocks like glucose, fructose and sucrose from sugar beets, sugar cane, wheat, corn, soy, etc.;
- second generation feedstocks like lignocellulose;
- dedicated feedstocks like pectin, chitin, alginate.

### *Why*

The main driver for the use of sugars as feedstock is feedstock diversification, but there is also a lot of potential towards reducing greenhouse gas emissions. On top of that, sugars are perfectly suited for fermentative and enzymatic processes, which have the potential to reduce GHG emissions even further. The potential (and the challenges), however, differ(s) between the different types of feedstock in combination with the processes to convert them in chemical building blocks.

Processes to produce first generation feedstocks – i.e. growing the crops and processing them into mono- and/or disaccharides at different levels of purity – are at full maturity and efficiency. Due to the high purity – albeit at a cost – the resulting mono- and disaccharides can be efficiently used in fermentation, enzymatic and/or chemical processes.

In the case of second-generation feedstocks, the opportunity mostly arises from the abundant availability of lignocellulosic side streams from, for instance, food processing companies at a low(er) cost compared to first generation feedstocks. The main challenges are related to getting the (hemi-) cellulose separated from the other components present in the lignocellulosic biomass, the effect of impurities on the conversion process(es) and finally the separation of the desired compound(s) from crude mixtures. And even more important doing all these steps in an economically viable way.

In both cases, added functionality compared to using fossil resources is mostly related to the conversion process(es) and less to the feedstock itself.

For dedicated sugar feedstocks, this added functionality is inherently present in the biopolymer itself. Challenges for the use of biopolymers like pectin and chitin are often related to the depolymerisation and/or modification to end-up with useful chemical building blocks. Drivers are again related to their availability as side streams from existing industrial activities, but in the case of chitin also from the dedicated rearing of insects using waste biomass as insect feed.

### *State-of-play*

Different projects related to the use of carbohydrate feedstocks have been or are running at Catalisti: Carboleum, CHITINSECT, Encaps2Control, SPICY, SweetEst and ATOL. These projects have already provided important results. At the same time, they have also shown the challenges that remain. Further research will be needed.

### *Next steps*

To boost the value of carbohydrate feedstocks, enabling setting up a full value chain, a number of important items need to be (further) developed:

- improving the robustness of both chemo- and biocatalytic processes for conversion of lignocellulosic biomass to cope with impurities;
- improving downstream processes to become more efficient in purification of the desired compounds;
- fully exploiting the added functionality that is inherently available and/or is created by conversion processes;
- combining chemo- and biocatalytic processes to leverage the functionality, robustness and overall efficiency of the carbohydrate-based value chain.

## Oils & fats

### *What*

Oils and fats are a generic term for (mixtures of) triglycerides, where the former are liquid at room temperature, while the latter are solid. The feedstock containing these oils and fats can be both vegetable and animal based. Vegetable oils are acquired from a whole range of different crops like rapeseed, sunflower seed, olive, maize and soybean, but also coconut and palm kernel to name a few. Animal based fats are typically acquired from livestock animals like pigs, chickens and cows, but can also be derived from other animals. Another source of ‘animal’ based fats is insect biomass. The triglycerides are typically composed of glycerol and fatty acids with different carbon lengths and degree of saturation.

### *Why*

Animal fats and oils are by-products from the animal rearing and meat industry. Inedible tallow is a major raw material source in the manufacture of fatty acids and hence in the production of oleochemical. Crops grown for vegetable oils on the other hand are typically grown specifically for its oils, leaving behind a solid protein-rich fraction used for animal feed and other purposes. Also here, the driver for the use of oils and fats lies with its abundant availability and hence its ability to substitute fossil-based resources. While the composition of oils and fats can be broken down to a limited number of common constituents, the combination of for instance the fatty acids with a broad range of (bio-based) alcohols and polyols leads to a vast number of different fatty acid esters serving a broad range of markets and applications.

### *State-of-play*

Oleochemistry is a well-established branch of biobased chemistry, serving markets like food and feed, surfactants and detergents, lubricants, coolants, but also covering biodiesel production. Even so, due to the virtually endless possibility to combine building blocks, the emergence of new building blocks and new types of catalysis, new ideas and products still pop up. Examples of oleochemical projects within Catalisti include Biovertol, PolyFlam and Encaps2Control.

### *Next steps*

Catalisti will continue to support projects that contribute to unlocking the full potential of this abundant biobased resource.

## Biomass side streams

### *What*

Biomass side streams can be defined as end-products of various processing industries that have not been recycled or used for other purposes. Examples include food processing residues, municipal organic waste or agricultural residues. These streams are typically composed of the formerly mentioned biobased resources like lignocellulose, sugars and oils & fats, but can for instance also contain proteins and inorganic matter. The efficient treatment of biomass side streams often requires a biorefinery concept (cf. lignocellulose processing) in which biomass side streams are pre-treated to extract valuable or inhibitory compounds or fractionated into their composing intermediates which are then further reconstituted to produce high-value industrial precursors, chemicals and energy. This concept uses an extensive range of technologies for the degradation and upgrading of biomass, including thermochemical, catalytic, fermentation and enzymatic processes.

### *Why*

Efficient transformation of biomass side streams to marketable products and energy contributes to a more circular economy. The major driver is to create more value for the biorefinery or processing industry. Other drivers are diversification of feedstock in the chemical industry, for example when extracting oils from food processing residues for use in cosmetics products, or finding a solution for a waste problem, for example the production of bio-methane from manure.

### *State-of-play*

To harness the maximum value from biomass side streams, it is essential to have knowledge of its chemical composition, including both the major and minor constituents. Most side streams are a complex and variable mixture of molecules, and pre-treatment becomes a key priority. A large number of technologies have been developed for the conversion of biomass to produce solid, liquid or gaseous biomolecules.

Developing a successful business case based on the valorisation of biomass side streams however, remains a challenge. Often, there is a mismatch between the cost of feedstock and treatment technologies and the potential market value of the products. Also, availability of streams is often disperse and fluctuating, implicating a complicated and therefore expensive logistics.

Different project related to this topic have been or are running at Catalisti, being Encaps2Control, ATOL, ValBran, Prometheus, Carboleum, CHITINSECT, AMBER and SUCCeSS. These projects aim to upgrade biomass side streams for different end applications and sectors.

### *Next steps*

Further research and innovation is needed for the development of more efficient separation and conversion processes and processes with fewer steps. Process intensification and continuous processes will be key to achieve more competitive, low CAPEX and OPEX technologies, that could enable successful business cases. Within Catalisti, we will work on membrane-based separations and chemical, physical and biotechnological solutions or sustainable combinations thereof. We will not focus on projects that mainly target energy valorisation of side streams.

## Chemical catalysis

### *What*

A catalyst is a substance which is added to a chemical reaction to increase the reaction rate, without being consumed during the reaction. In contrast to enzymatic catalysis, chemical catalysis refers to the use of chemical compounds as catalysts, with metal-catalysed reactions (often transition metal or transition metal complexes) and acid and base catalysed reactions as well-known examples. Furthermore, catalytic reactions can be divided into two main types: heterogeneous catalysis (catalyst in a different phase than the reactants) and homogeneous catalysis (catalyst in the same phase as the reactants).

### *Why*

The transformation of biomass into a variety of useful biobased compounds requires efficient methods and chemical catalysis is often required for reactions to take place at reasonable rates. In comparison to enzymatic catalysis, chemical catalysis usually relies on more active and robust catalyst systems and can handle varying and challenging feedstocks as well as more adverse conditions. Moreover, following the initial (catalytic) conversion of biomass into building blocks, chemical catalysis is a useful and versatile technology to modify building blocks into industrially relevant end-products.

### *State-of-play*

Chemical catalysis has a long history in the chemical industry. Nonetheless, knowledge is still being generated by research into new catalyst systems, for new or more efficient biomass conversions, or by increasing the understanding of the mechanisms of catalysed reactions. A number of Catalisti projects have been and are running with focus on chemical catalysis, such as ARBOREF, BIORESAL, Biovertol, Bio Wax, Carboleum, Encaps2Control, MAIA, PolyFlam and SPICY.

### *Next steps*

In line with SusChem SIRA, where chemical catalysis is labelled a technology priority, Catalisti will continue to support innovation projects with a focus on chemical catalysis. Advances in research on chemical catalysis with relation to biomass include enhancing biomass catalysis valorisation, such as biomass liquefaction, the catalytic upgrading of fractionated lignocellulose and the conversion of biomass to synthesis gas for the production of fuels and chemicals.

## Enzymatic catalysis

### *What*

Enzymatic catalysis (or biocatalysis) refers to the use of enzymes (isolated enzymes or whole cells) to catalyse chemical reactions. Enzymatic reactions are typically equilibrium reactions, and thus reversible. Depending on the type and direction of the reaction (e.g. condensation vs. hydrolysis), reactants need to be replenished and/or reaction products need to be removed. Some enzymes also need co-factors to be able to exhibit functionality. As with metal catalysts, isolated enzymes can be used as catalysts as such, but also immobilized on a carrier material.

### *Why*

To convert biomass (and other feedstocks) into useful building blocks, enzymatic catalysis is a key component in the conversion toolbox. Compared to metal catalysts, enzymes can have advantages in terms of faster reaction rates and milder reaction conditions (temperature, pH, …). Yet, the biggest driver of enzymatic catalysis is the ability to reach high(er) and even other selectivities, for instance chemo-, regio-, diastereo- and enantioselectivity, but also higher purities and yields, compared to conventional (chemocatalytic) means.

### *State-of-play*

Enzymatic catalysis has been used already for decades in the chemical, pharmaceutical, agricultural, food, feed and cosmetic industries. Typical biotransformations include transesterification, hydrolysis, oxidation, reduction, addition – elimination, halogenation and dehalogenation reactions. Different projects related to enzymatic catalysis have been or are running at Catalisti, like EnzymASE, Lipametics, SweetEst. These projects are exploiting the drivers mentioned above.

### *Next steps*

According to SusChem SIRA, the challenges and goals to boost the use and added value of enzymatic catalysis, and industrial biotechnology in general, are amongst others related to the following items:

- identification and engineering of more active and robust enzymes;
- development of bioplatform technologies for improved enzyme strain engineering (e.g. improved '–omics' methods for system understanding, high-throughput engineering, high-throughput screening);
- integrated optimisation and development of metabolic engineering, pre-treatment, bioconversion, product recovery and downstream processing;
- development of realistic models of the production process and realistic models of reactor types equivalent to the computational systems already used in other engineering fields;
- development of combined chemo-bio-processes looking at novel ways in which bio- and chemo-catalysis steps can be combined to improve process economics (and added functionality).
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Flanders has a lot of expertise in the field of enzymatic catalysis and industrial biotechnology in general, both at research institutes and companies. The challenges defined by SusChem SIRA correspond very well to the hurdles our stakeholders highlighted based on project results and other experiences.

## Fermentation

### *What*

Fermentation is a metabolic process that breaks down biomass by enzymatically converting the sugars present in biobased feedstock into alcohol or acid. For this purpose, yeast or bacteria are added to the feedstock. Biomass pre-treatment can be required to liberate sugars present in different types of biobased feedstocks. Yeast and microbial strains can be tailored via strain engineering and optimisation, to allow the production of different chemicals from various feedstocks at relevant product tiers. Downstream processing and in-situ product recovery are a crucial aspect of fermentation technology, as it allows to separate and purify the synthesized biobased chemicals from the fermentation broth.

### *Why*

The main driver for fermentation technology is that it allows the direct transformation of sugar-containing feedstock into rather complex molecules. This differs from enzymatic catalysis, where the enzyme first needs to be expressed in a specific strain and then isolated. Furthermore, by means of strain engineering and expression of multiple enzymes, consecutive conversions can take place in the same fermentation medium. Most fermentation processes are taking place in mild conditions such as temperatures close to ambient, which are compatible with living yeast or microbial strains, making fermentation technology a rather energy-efficient process.

### *State-of-play*

The end-markets of the fermentation industry range from pharmaceuticals, food, feed and fuel to chemical building blocks. Some fermentation processes are longstanding industrially validated processes, such as the production of bioethanol from sugar cane and sugar beets. Other fermentation processes are still in an earlier phase, where additional research is required. A large variety of functional molecules is accessible via fermentation pathways, given the required strain development research, optimization of processing conditions and recovery and purification methodologies. Catalisti projects which include fermentation research and are directed towards various applications are AppliSurf, ARBOREF, Prometheus and SPICY.

### *Next steps*

Fermentation is considered an important technology within industrial biotechnology and is named by SusChem SIRA as one of the advanced processes to contribute to the energy transition and circular economy of the future. Increased versatility of fermentation processes (using different feedstocks, enabling the production of various biobased chemicals) will help advance this technology. Even more crucial are challenges related to production yields, in particular when upscaling to industrial scale and efficient separation and purification methods at larger scales.

## Biobased end-products

### *What*

Products and materials are labelled biobased when they are made from biomass feedstock and therefore contain renewable carbon. There is no additional differentiation based on the type of conversion technology used for the required transformations. The variety of biobased end-products, materials and their applications is very large, with some major product categories being dispersants, emulsifiers & encapsulants, lubricants, surfactants and biobased resins. Both drop-ins or analogues of fossil-based structures can be obtained from biobased feedstock, as well as entirely new molecular structures, by utilizing the functionalities intrinsically present in different types of biomass.

### *Why*

Most sectors are experiencing an increasing drive towards sustainable alternatives for their fossil-based materials and products. The main drivers here are generally the limits of fossil resources and the impact of their use on the climate and the environment. Additional legislative drivers may apply for specific markets and applications, as well as market push, when costumers are requesting biobased alternatives. Additionally, the functionalities and chemical structures available in, or through, biobased feedstocks create opportunities for the development of new molecular structures, with functional groups which are often not accessible in fossil-based resins, in turn creating new properties and opportunities.

### *State-of-play*

The large variety of end-products translates to different TRL levels. For some products and product categories, industrial implementation is ongoing or established, while others still require extensive research. Some examples across the TRL scale are: bio-ethanol for fuels (currently already available on the market), biolubricants derived from vegetable oils as transmission fluids (TRL 7-8), biosurfactants in applications across pharmaceutical, cosmetics, and textile industries (TRL 7), PHAs from urban wastes or renewable oils and fats for packaging materials and biomedical applications (TRL 6), bio-composites such as PLA or PHA reinforced with natural fibres (TRL 5), lignin oil as platform chemical for a wide variety of products such as added-value carbon-based materials (TRL 4-5), fine- and specialty chemicals and chemical feedstock in general (TRL 4-5).

The majority of projects in the Catalisti portfolio, and especially those within the innovation program Biobased Value Chains, are value chain projects that often involve multiple end-users, testing the potential of biobased products and materials for their target applications. Some examples of projects focusing on the aforementioned product categories are:

- dispersants, emulsifiers & encapsulants: CHITINSECT, MAIA
- lubricants: Lipametics, PolyFlam
- surfactants: AppliSurf, Biovertol, Carboleum
- resins: MAIA, CHITINSECT and AMBER

***Next steps***

Within Catalisti, there is still a large potential for additional projects developing biobased end-products. They can have several points of focus, depending on the needs and wishes of the industrial partners.

## Link with other Catalisti programs

Biomass side streams
→ link with CRE

Technologies for biomass conversion like chemical and enzymatic catalysis as well as fermentation
→ link with PIT

Development of new biobased products like surfactants and lubricants
→ link with ASP

## Link with Moonshot Research Trajectories

Strong link with MOT1 Biobased Chemistry. Follow-up trajectories of successful MOT1 projects can fit in this program.

## Active companies

Companies active in projects within the BVC innovation program include, but are not limited to: 3M, Ajinomoto BioPharma Services, AVEVE, B4Plastics, Beaulieu, Boss Paints, Calidris Bio, Cargill, ChemStream, Circular Organics, Citrique Belge, Cobalin, Devan, Eastman, Eco Treasures, Ecover, Genano, Globachem, Gova, Govi, Group Depre, I-Coats, INEOS, InOpSys, Kingspan, Lawter, Nutrition Sciences, Oleon, Proviron, Purazur, Recticel, Rendac, Sappi, Soudal, SPAAS, Suez, Sumitomo Bakelite, Tectero, and Transfurans Chemicals.

# Process Intensification and Transformation (PIT)

## What

In this innovation program, we focus on the innovation of chemical processes. These innovations can be incremental, i.e. improvements of existing processes or new ways to perform existing processes, as well as radical, i.e. breakthrough innovations leading to completely new processes. Therefore, we call this program “process intensification and transformation”.

Process intensification is mainly focussed on energy efficiency, resource efficiency, the reduction of waste, and process safety. We look at technologies like flow chemistry, energy-efficient separations, new reactor design, alternative solvents or waste-heat recovery. Besides the improvement of individual processes, the integration of processes is important too. This will result in processes that are safer, cleaner, smaller and cheaper.

In addition, we work on more radical process transformations that will enable the use of renewable energy in our processes like electrification and adaptation to variations. We also work on Carbon Capture & Utilization (CCU) and look at the cost-effective production of hydrogen and its potential as a chemical feedstock. In the field of renewable energy and energy carriers (hydrogen can also be used as an energy carrier), the chemical sector is not in the driver seat, but as a major energy user and provider of technological solutions, the chemical sector plays an important role in this evolution.

Digitalisation as a major driver of innovation plays an important enabling role in this program. New digitally enabled solutions improve process control and operations’ efficiency and reliability. These new solutions can further optimise the processes, for example through sensors, model predictive control and predictive maintenance. In addition, these new solutions can also improve production management, for example by considering product quality, as well as the energy and resource efficiency of connected processes and plants.

## Why

The improvement of processes in the chemical industry, to reach better energy and raw material use efficiency, is important both from an environmental and an economic perspective. Continuous incremental improvements of processes are crucial to achieve an environmental footprint that is as low as possible, as well as a competitive position compared to the rest of the world.

We also work on more radical transformation of processes in the chemical industry, as this will be needed to realize significant greenhouse gas emission reduction and avoidance in our own sector as well as in other sectors, which will ultimately contribute to reaching the climate goals. Furthermore, new processes will be needed for the realization of a circular economy.

## Goals

The goal of the Process Intensification and Transformation program is to, each year, develop several improved processes that are safer, save energy, save resources, produce less waste, are more flexible, and/or deliver higher quality.

In addition, in the longer term, we want to develop a number of radically new processes that not only enable the sustainable transformation of the chemical industry, but - through its services and products - also the sustainable transformation of other industries. This way, the chemical industry will take on a crucial role in the sustainable economy and society of the future.

Every project within this program has the clear ambition to deliver one of the following:

- an improved production process in the chemical value chain that contributes to both increasing the economic and decreasing the environmental impact of the current process; or
- a crucial step forward in the development of a radically new process, which in turn will contribute to the sustainable transformation of our sector (as well as other sectors).

# Topics

## Continuous processing

### *What*

In continuous (flow) processing, a chemical reaction is run in a continuously flowing stream rather than in batch production. In other words, pumps move fluid into a tube, and where tubes join one another, the fluids come into contact with one another. If these fluids are reactive, a reaction takes place. Continuous processing is a well-established technique for use at a large scale when manufacturing large quantities of a given material (e.g. as in the petrochemical industry). However, continuous processing is a new concept in the pharma industry, which was founded using a batch production approach. It is also being contemplated at a time when the demand for large-volume manufacturing is shrinking, because blockbuster drugs are being replaced by small-volume, highly potent, complex drug substances that make the effective use of continuous processing more challenging. In the pharma industry, the term 'flow chemistry' has only been coined in the last decade for its application on a laboratory scale. In this case, so-called 'microreactors' are used.

### *Why*

Continuous processing has several advantages, such as cheaper labour rates since production will rely mostly on machinery than any other resource, minimization of waste and high return on investments. Other main drivers for implementation are the improved safety, higher and constant quality, increased competitiveness (due to increased raw material and energy efficiency), shorter time-to-market, easier scale up, and the opportunity to benefit from new process windows (time, temperature, pressure, etc.). Combining continuous flow unit operations with batch reactors can also prove to be very valuable as a process intensification strategy. For instance, using membranes in reacting batch systems provides a combination of diverse functions that can lead to significant improvements in the process performance. Those improvements include, among other things, better yields/selectivities (e.g. via equilibrium shift), better energy management, more compact design, extension of catalyst lifetime, etc.

### *State-of-play*

The Catalisti project portfolio contains various projects where predominantly flow chemistry has been the main research focus, ranging from researching different types of reaction conditions on lab scale (e.g. multiphase, highly-exothermic reactions) over modelling efforts (to gather the design input needed for the development of a multipurpose pilot plant flow reactor) to researching scale up. In some of these projects, research is also performed on the synthesis of organic micron-sized crystals of active pharmaceutical ingredients, nano dispersions of coating resins and microcapsules with active ingredients. This in order to overcome current limitations in heat and mass transfer, which result in little control over the average particle size, particle size distribution and batch to batch variations. Some projects in the Catalisti project portfolio are: ATOM 1, ATOM 2 and PIF. These projects typically target TLRs of 4-5.

### *Next steps*

The latest SusChem SIRA confirms the importance of further R&D&I actions in the field of continuous processing and flow chemistry. Some specific challenges that are frequently mentioned are:

- improved energy and resource efficiency in the chemical industry, through higher conversion rates and selectivity of reactions, operating in a continuous mode at different scales;
- development of suitable membranes that exhibit sufficient selectivity, permeability and stability (incl. inorganic (ceramic or metallic) and polymer membranes) to be used in membrane reactors;
- development of approaches for fast determination of kinetics (by characterization of fluid hydrodynamics and heat & mass transfer);
- new scalable designs of clogging-resistant continuous flow reactors for process intensification;
- rational scale-up of continuous flow reactors (accounting for temperature spikes and using model-based development);
- integration of suitable sensors in microreactors for online analytics;
- development of modularized ('plug & produce') production plants;
- development of new reactor and process design utilizing non-conventional energy forms (e.g. plasma, ultrasound, microwave, photochemistry);

- making more use of the benefits that digitalisation can bring to flow chemistry.

Within Catalisti, we will continue to extend the knowledge base on continuous processing and flow chemistry in Flanders and increase its applicability in industry by supporting applied research as well as pilot projects.

## Separation processes

### *What*

The functions of separation processes typically include the removal of impurities from raw materials, products, and by-products; the separation of recycle streams; and the removal of contaminants from air and water waste streams. Separation processes are often classified according to the particular differences in chemical properties or physical properties they use to achieve separation of the constituents of a mixture, such as size, shape, mass, density, or chemical affinity. If no single difference can be used to accomplish the desired separation, multiple operations combined can often achieve the desired result.

Separation processes are of great economic importance to the chemical, petroleum refining, and materials processing industries as they are accounting for 40-90% of capital and operating costs in industry. Nonetheless, separations are often overlooked and underappreciated.

### *Why*

Traditional separation technologies, such as cryogenic distillation and solvent extraction, are energy-intensive and cause serious environmental stress. Advanced separations and further innovation in this area are thus required to significantly reduce energy usage and hence operating costs of separation processes. Indeed, to be globally competitive and to meet numerous emerging challenges, the EU manufacturing industries will have to be both resource and energy efficient. Continuous improvement in product quality along with flexibility in production processes and product mix is essential. Conforming to rigorous safety, health and environmental regulations has become crucial. To approach the aspirations of the future, industrial parties will have to dare to thoroughly re-evaluate their production and separation processes. The development and optimization of innovative separation technologies that lead to ‘process intensification’ opens the road to a more sustainable method of production.

### *State-of-play*

In this philosophy of process intensification and energy-efficient separation processes, there are some separation technologies that can play an important role. Particularly membrane technology, adsorptive porous materials and the application of alternative or additional forms of energy in separation processes offer great potential.

1) Membrane technology
   Membrane technology can have an important role. In general, membrane processes do not demand a phase transition by which high energy costs are avoided. Moreover, the mild temperatures result in a higher product quality in case of purification of thermally labile molecules and in a safer processing. It is also possible to recycle raw materials, process water and solvents from process and waste streams. Thanks to their modular architecture, the membrane processes are easily scalable and can be compact, when they are based on membrane modules with a high surface-to-volume ratio.

   More specifically, organic solvent nanofiltration (OSN) offers an economically interesting, alternative separation process that has the added advantage of often leading to a more sustainable process. Allowing non-thermal, energy-efficient and highly selective separation, OSN has the potential to replace part of the huge number of traditional, mainly thermal separation processes currently used in the chemical and pharmaceutical industry. Some example projects on OSN/membrane technology in the Catalisti project portfolio are the ICON project SuMEMS and the SBO project EASiCHEM.

2) Adsorptive porous materials
   Among all the mixtures, the separations of gas mixtures are of great importance in industry, such as $CO_2$ capture ($CO_2$/air, $CO_2$/$H_2$), natural gas sweetening ($CO_2$/$CH_4$, $N_2$/$CH_4$, $H_2S$/$CH_4$),

$O_2$ purification ($O_2/N_2$), light hydrocarbon separation (olefins/paraffins, linear/branched isomers, etc.), noble gas separation and so on. For these mixtures, the gases are in a similar molecular size, or their physical properties are close, making their separation difficult and energy intensive.

A viable green alternative for the efficient separation of relevant gases (in order to mitigate the pressing issue of minimizing the sky-soaring energy expenditure) could be the use of advanced adsorptive porous materials, such as, metal-organic frameworks (MOFs). MOFs are attractive in gas-separation applications on account of their large surface areas, adjustable pore sizes, highly predictable and variable structures. Currently, no projects in the Catalisti project portfolio have a central focus on MOFs/adsorptive porous materials.

3) New Developments in High-Gravity (HiGee) Technologies
In the chemical industry, the demand of more flexible apparatuses and innovative production concepts offering significant improvements in terms of energy efficiency and sustainability increases remarkably in recent years. To meet this demand, different approaches based on the application of alternative or additional forms of energy or on the change and improvement of structural parameters are investigated. An alternative and very promising technology is 'High-Gravity (HiGee)' technology (centrifugal mass transfer contactor), in which a centrifugal field is applied to improve the performance of mass-transfer processes.

High-gravity technology is an enhanced transmission and multi-phase reaction breakthrough technological process. In the high-gravity environment, molecular diffusion and mass-transfer processes between the molecules in the different phases are much faster than in a conventional gravity field. The easiest method to achieve a high-gravity environment is to generate centrifugal force by rotation. HiGee technology has been successfully applied to gas/liquid reactions in the chemical industry and has been extended to liquid/liquid application fields, such as micro-mixing, emulsification, extraction, liquid membrane separation, chemical reaction, and other domains. Currently, no projects in the Catalisti project portfolio have a central focus on HiGee technologies.

***Next steps***
Catalisti will initiate and elaborate new projects on energy-efficient separation processes. Regarding the three example separation processes mentioned above, the following issues will (need to) be addressed:

1) OSN/membrane technology
To profit from the full potential of OSN, however, some remaining challenges and market demands need to be solved. Nowadays, the main challenges related to the development of membrane processes for OSN are (i) the robustness of the membrane materials in organic solvents, in harsh acid and basic conditions, and during module preparation; (ii) the robustness of the membrane materials toward swelling and leaching; (iii) the lack of "multipurpose membranes"; (iv) the membrane selectivity for challenging molecular separations, as in the case of mixtures of main products and impurities with similar molecular size or for mixtures of isomers; and (v) the capability to describe/predict NF performance by means of modelling tools and to carry out process design. On the market demand side, a more extensive demonstration of the technology by relevant pilot testing is wanted because it is common practice that end-users only choose for new developments that have been already implemented at reference sites, or at least technically proven at larger scale. This also requires the proper upscaling of OSN-membranes, that have been proven valuable on the lab-scale.

2) MOFs
Different from inorganic solid adsorbents, such as zeolites, inorganic oxides, and porous carbon-based materials, MOFs consist of inorganic metal ions or nodes connected by organic ligands, offering sites for both organic and inorganic chemistry within their pore. The organic linkers can be modified with functional groups to tune the electric potential of pore surface, and some MOFs have open metal sites (OMSs) and these OMSs can be chosen judiciously for desired applications. There are virtually endless possibilities of making this type of porous materials by the combination of these inorganic nodes, organic linkers, and functional groups

in framework structures of different topologies, which would be promising for the fulfilment of some important and challenging applications.

3) High-Gravity (HiGee) Technologies
   Advantages of HiGee technologies are modularity, high flexibility, intense mass transfer and very compact design resulting in potential savings in operation and investment costs. Many chemical processes could benefit from these unique properties by reducing the cost of construction, reducing working capital, improving safety, producing less waste, etc. In addition, the use of HiGee fields may provide solutions to processing problems more effectively and more economically than conventional equipment. However, a deeper understanding of the process fundamentals and of the most essential process variables must be gained to provide a sound basis for understanding the performance enhancement available to a wide variety of applications. This will be extremely helpful to set the boundaries for use of HiGee technologies in chemical processing.

## Electrochemical processes

### *What*

Electrochemistry studies chemical reactions which take place at the interface of an electrode and an ionic conductor, the electrolyte. These reactions involve electric charges moving between the electrodes and the electrolyte (or ionic species in a solution). As such, electrochemistry deals with the interaction between electrical energy and chemical change. When a chemical reaction is caused by an externally supplied current (as in electrolysis), or if an electric current is produced by a spontaneous chemical reaction (as in a battery), it is called an electrochemical reaction. In electrocatalytic processes, carbon-based electrodes are combined with different catalysts like electrocatalysts, enzymes or biocatalysts as whole cells. If in addition, light is used to power the electrocatalytic reaction, we speak about photo-electrocatalytic processes.

### *Why*

Electrochemical processes can provide new production routes for various chemicals. They can give rise to inherently safe processes, reduce the number of steps, allow for milder reaction conditions, generate less waste due to their unique reactivity and provide alternative routes to access desired structural entities.

Electrochemistry also provides opportunities for sustainable energy use in chemical production. Novel electrochemical processes can enable climate-neutral synthetic routes by exploiting new reactivities that enable molecular transformations difficult to realise via thermochemical methods. Hydrogen production, the utilisation of alternative carbon feedstock (waste, biomass, $CO_2$), waste treatment or catalyst recovery are promising applications of electrochemical processes.

### *State-of-play*

Current applications for electrochemical production of bulk chemicals is still limited to a few and long-established electrolysis processes like chlor-alkali electrolysis. For fine chemicals production, electrochemical and photochemical reactions are used in very specific cases, and mostly on a small scale.

The Catalisti project portfolio currently does not include projects that focus on electrochemical, electrocatalytical and photo-electrocatalytical processes. However, some specific electrochemical and photochemical reactions are included in the ATOM and the PIF projects as case studies for research on flow chemistry.

### *Next steps*

Catalisti will further explore the potential of electrochemistry for different reactions, from the production of fine chemicals over the production of hydrogen to the valorisation of alternative feedstock like biomass and $CO_2$. For the latter, more efforts are needed to control the interface between electro-catalyst, electrolyte and in case of $CO_2$ feedstock also gaseous reactants (development & improvement of gas diffusion electrodes).

## Carbon Capture and Utilization (CCU)

### *What*

CCU is a broad term that covers all established and innovative industrial processes that aim at capturing $CO_2$ – either from industrial point sources or directly from the air – and at transforming the captured $CO_2$ into a variety of value-added products such as synthetic fuels, chemicals and building materials. Most reactions to transform the $CO_2$ molecule require an additional energy input, which must come from a sustainable low carbon source. Other terms such as $CO_2$ transformation, $CO_2$ conversion, $CO_2$ recycling, $CO_2$ valorisation, or $CO_2$ upcycling can also be used.

### *Why*

CCU technologies offer a number of opportunities for European industry and the pursuit of EU policy objectives, including:

- supporting decarbonisation of the EU energy system and turning the industry climate neutral;
- supporting the circular economy, by converting waste $CO_2$ to products, industrial innovation and competitiveness, particularly important for energy-intensive industries, developing new and more efficient processes and creating new market opportunities;
- supporting energy security and renewable energy deployment, through utilising excess renewable electricity and providing energy storage alternatives and through the development of new climate neutral fuels (synthetic methane, ethanol, methanol, …).;
- supporting the evolution of $CO_2$ capture systems, which may help deployment of Carbon Capture and Storage (CCS) technology, which in turn provides permanent and large-scale storage of $CO_2$.

### *State-of-play*

The CCU field is heterogeneous, covering a wide range of technologies and products, and a wide range of diverse actors and industries. CCU technologies are at different stages of technological readiness, from laboratory testing to pilot scale and commercial demonstration (Power to methanol, Dream Reaction) and still face a number of technical challenges. There are also barriers to CCU implementation, among others the energy cost associated with the unfavourable thermodynamics of many conversions and supply capacity, both in terms of co-reactants in any process and also in market demand for the product. The current Catalisti project portfolio consists of two projects: $CO_2$PERATE (cSBO, TRL 2-4) and CAPRA (ICON, TRL 4-5). While $CO_2$PERATE mainly focuses on the generation of a sound knowledge base for benchmarking, developing and comparing various technologies for the direct conversion of $CO_2$ to formic acid using catalysis and renewable energy, CAPRA aims to upgrade the effluent resulting from fermentation process using exhaust gases emitted by the steel industry to a medium-chain carboxylic acid bio-oil.

### *Next steps*

Advancement of knowledge is essential to improve the economic and environmental feasibility and the potential of the technologies. This includes – among others – more R&I activities on:

- the collection and purification of $CO_2$ from a variety of sources;
- the synthesis of climate friendly hydrogen via water splitting powered by climate neutral energy sources, by pyrolysis of methane or other climate friendly productions methods;
- catalyst design with increased activity, stability, selectivity and tolerance to poisoning and if needed, for low-temperature operations,
- reactor design and engineering to achieve improved reaction control;
- demonstration at large scale and in different settings.

The result of the implementation of CCU are often molecules that are identical as or have to replace existing molecules meaning they have to compete with existing prices. Cost reduction is therefore an absolute priority for future innovation.

## Hydrogen

### *What*

Hydrogen is considered a valuable molecule which has multiple applications, both in industry and in the energy system. In the chemical industry, hydrogen is an important feedstock to produce valuable chemicals, such as ammonia and methanol. Reactions with mixtures of hydrogen, carbon monoxide and carbon dioxide are well known as synthesis gas-based routes, and they can be used to build-up all major platform chemicals for the chemical industry's value chain. In refineries, hydrogen is used for hydrogenation processes, which are commonly employed to saturate organic compounds. In the energy economy, hydrogen is expected to play a key role as an energy carrier in future energy systems of the world.

### *Why*

Achieving a low-carbon chemical industry requires process intensification and transformation of hydrogen production, thereby shifting from the fossil-based Steam Methane Reforming (SMR) to new, low carbon technologies such as electrolysis. Hydrogen acts as a key high-energy containing reaction partner in the conversions of $CO_2$ to the aforementioned platform molecules. In these conversions, hydrogen delivers the energy necessary to activate and convert both the kinetically inactive and thermodynamically stable carbon dioxide molecule. As energy carrier, hydrogen can play a significant role in decarbonizing the world energy supply to mitigate climate change. Therefore, a major change in the energy economy from fossil energy carriers to renewable energy carriers is necessary.

### *State-of-play*

Today, hydrogen is predominantly produced from natural gas using SMR, which is responsible for about 3% of global industrial $CO_2$ emissions. Additionally, hydrogen is also produced as a significant side stream of other reactions like dehydrogenation processes and chlorine production. One approach could be to reduce the $CO_2$ emissions of SMR by developing and implementing Carbon Capture & Storage (CCS) and Carbon Capture & Utilization (CCU) technologies.

Another approach could be to produce hydrogen using low carbon technologies, e.g.:

- Water electrolysis: water is split into its elements, i.e. hydrogen and oxygen, by applying an electric current. The $CO_2$ footprint of this hydrogen production via electrolysis rests essentially with the $CO_2$ emissions of the respective power generation process. Therefore, none of these routes will have a positive impact on the overall $CO_2$ emissions, unless the electricity used is based on low-carbon power generation.
- Photo-electrocatalytic (PEC) hydrogen production: hydrogen is produced from water using sunlight and specialized semiconductors called photoelectrochemical materials, which use light energy to directly dissociate water molecules into hydrogen and oxygen.
- Pyrolysis of methane: methane is split into hydrogen and solid carbon. This methane pyrolysis process requires little energy compared to water electrolysis. If the process is based on climate neutral energy, hydrogen could be produced on an industrial scale without $CO_2$ emissions, even when using fossil-based methane as a starting material.
- Dry reforming of methane (DRM): the process of converting methane and carbon dioxide into synthesis gas (syngas, $H_2$ + CO), an important building block for world scale industrial processes and energy conversion.

### *Next steps*

Hydrogen will play an import role in the future as a feedstock and as an energy carrier. Therefore, all production methods of climate friendly hydrogen are considered as a potential subject for research. As a major user of hydrogen as feedstock and potentially as energy carrier, and as supplier of technological solutions, the chemical sector will play an important role in this evolution. Cost reduction (CAPEX & OPEX) and improving the performance of climate friendly hydrogen production, through e.g. catalyst development, materials & system integration and the availability of low carbon electricity, is therefore an absolute priority for future innovation to compete with current sources of energy production.

## Energy efficiency & electrification

### *What*

In the last two decades, the European chemical industry has put tremendous effort in improving its energy efficiency, resulting in about 22% less fuel and power consumption. Further measures to reduce the carbon-intensity of energy consumption may include incremental energy efficiency improvements, the direct use of low carbon electricity for heat generation, the use of new energy carriers for heat generation and the electrification of chemical processes. Additionally, energy flexibility in terms of demand side management can be used to valorise intermittent surplus supply of renewable electricity. This way, the chemical industry can benefit from periods with low electricity prices, the stability of the energy system will be positively affected and the available energy is consumed more optimally. For the indirect use of electricity to produce hydrogen and subsequent conversion with $CO_2$, the reader is referred to the CCU topic.

### *Why*

Despite abovementioned efforts to reduce fuel and power consumption, the energy demand of the chemical industry remains enormous, resulting in significant emissions of $CO_2$. For example, the generation of heat by combustion of natural gas, which accounts for 60% of the total fuel used, corresponds to 17.8 Mt $CO_2$ emissions on a yearly basis for the European chemical industry. Therefore, incremental energy efficiency improvements, shifting from fossil-based fuels to the direct use of low carbon electricity for heat generation and the electrification of chemical processes are crucial to achieve an as low as possible environmental footprint.

### *State-of-play*

Chemical companies contribute by incrementally boosting the energy efficiency of their processes by more selective, active and/or durable catalyst systems, optimised reactor performance, higher levels of heat integration, improved operating conditions, etc. Typical process-intensifying equipment encompasses intensive mixing, heat and mass transfer devices including structured reactors, advanced heat exchangers and enhanced (HiGee) or cold (e.g. membrane) separation equipment as well as integrated hybrid equipment such as reactive distillation, heat exchange reactors and membrane reactors.

SPIRE estimated 20–50% of the energy used in industrial processes to be lost as exhaust gases, cooling water and heat losses from equipment and products. For the large petrochemical processes, a high level of heat integration on plant and site level has usually been achieved, deficits exist more for smaller, isolated installations, and low-to medium production processes, which are often realized in batch processes. VoltaChem, a Shared Innovation Program that connects the electricity sector, equipment sector, and chemical sector, estimates that about 35% of the final energy use for heat in the chemical industry is for heat at temperatures up to 200°C. A promising approach to reach industrial relevant temperatures up to 200-250°C is to upgrade residual heat streams with ‘power to heat’ technologies, e.g. new innovative heat pumps and mechanical vapor recompression (TRL6-7). Alternatively, residual heat streams could also be valorised by ‘heat to power’ technologies to convert heat in electricity, such as thermoelectrics, which are still at TRL 5-8.

Energy-intensive chemical processes, e.g. olefin production by steam cracking and ammonia production via the Haber-Bosch process, are major contributors of the $CO_2$ emissions in Flanders. These processes rely respectively on the combustion of fossil fuels to heat furnaces and fossil fuels as a feedstock for hydrogen production. Therefore, the electrification of these processes, i.e. for heat generation or hydrogen production, is a promising approach to reduce greenhouse gas emissions but is still on a low TRL and would require large amounts of electricity.

### *Next steps*

Further energy efficiency improvements can be reached through process intensification and transformation, by the optimization of heat integration and the valorisation of residual heat. The latter can be done in terms of ‘power to heat’ for upgrading low temperature waste heat streams and ‘heat to power’ to produce electricity out of waste heat streams. More fundamental and disruptive breakthroughs (TRL1-3) regarding the development of ‘power to heat’ and ‘heat to power’ technologies and the electrification of chemical processes are expected to initially take place in the Moonshot initiative and subsequently to be transferred to the regular Catalisti operations in terms of industry-driven follow-up projects.

## Digitalisation

### *What*

The chemical and plastics industry is confronted with a new type of industrialization: Industry 4.0 (I4.0). In essence, I4.0 stands for the arrival of the internet on the production floor. It involves the integration of digital technologies and automation into production and logistics and the use of Industrial Internet of Things (IIoT), data analytics and digitized services in industrial processes. I4.0 offers interesting opportunities to better respond to customer requirements through automation, digitization and interconnectedness between products, value chains and business models.

***Why***

Digitalisation accelerates innovation, increases productivity, spurs growth, and leads to more efficient and effective management practices. It also contributes to sustainability goals by enabling sustainable production, reuse, and recycling of chemicals and plastics, decreasing waste generation, as well as reducing energy, solvent, water and/or raw material usage. In short, digitalisation delivers chemical companies a competitive edge on multiple fronts.

Digitalisation is of high interest to chemical companies in Flanders. However, this does not (yet) translate in the degree of implementation of I4.0 within these companies.

***State-of-play***

Today, many advanced digital technologies have reached a cost and performance level that enables their application in chemical production and process environments. Across the sector, cautious digitization steps can already be observed. Yet, this does not represent the revolutionary shift necessary for a complete digital transformation of chemical production or process environments. Part of the reluctance of the chemical sector is related to safety aspects. However, the main barrier for the integration of digital technologies in industrial processes are the lack of success stories, which leads to a “wait-and-see” attitude in many chemical sector companies. Indeed, for many companies, I4.0 is a major challenge with many hurdles and unanswered questions. Digitization can be highly advantageous in R&D environments, HR, supply chain and logistics. Yet, according to Catalisti’s DigiChem study, the major interest within the chemical industry relates to process optimization (optimized energy usage, predictive maintenance, minimizing raw material use and waste). Self-optimizing processes rely on data. Consequently, I4.0 topics associated to digitalisation include data generation, data valorisation, data basing, data processing and decision making. There is still a big challenge in setting up a good interface between all existing equipment and systems. Not all equipment can be easily connected (e.g. some legacy machines need to be equipped with smart sensors to be able to connect them with other entities: cyberizing legacy equipment). Additionally, different IT applications need to be integrated in such a way that optimized data exchange can be done. This interconnectivity is a basic requirement to start with I4.0, in which IIoT will become of increasing importance. Upon successful rollout of IIoT, data isolation and valorisation will be the real challenge. Many companies fail to take advantage of data and the potential intelligence these data possess. AI/ML expertise within companies is very scarce. When being present, it is still in a very early, explorative stage. This because AI is a very broad domain, which makes it impossible e.g. for a process engineer, but also for a data scientist, to be an expert on all sub aspects. Moreover, optimal implementation of AI-technology, requires multidisciplinary talent with insights in both chemical engineering and data science. Only then, a company's business challenge can be successfully translated into AI. The capability to translate technological needs into what a data scientist should do is currently the major bottleneck for the digitalisation of companies.

***Next steps***

There are many companies in Flanders (including start-ups and scale-ups) that can offer expertise in data analysis. It is, however, important to include domain-specific expertise (e.g. chemistry knowledge), and not only the knowledge to process data (e.g. mathematical algorithms). Flemish companies and knowledge institutes offer expertise in both fields. Bringing the multi-disciplinary expertise together and translating their capabilities and needs is a crucial step to further increase the level of digitalisation knowledge and expertise in Flanders.

## Link with other Catalisti programs

Intensification and transformation of biobased conversion processes
→ link with BVC

Reduction of waste
→ link with CRE

Carbon Capture & Utilization
→ link with CRE

Safer processes
→ link with ASP

Digitalisation
→ enabler in all three other programs

## Link with Moonshot Research Trajectories

This program has a partial link with MOT3 Electrification & Radical Process Transformation and with MOT4 Energy Innovation. Follow-up trajectories of successful MOT3 (and MOT4) projects can fit in this program.

## Active companies

Companies active in projects within the PIT innovation program include, but are not limited to: 3M, Agfa, Air Liquide, Ajinomoto BioPharma Services, Allnex, BASF, Borealis, Cronos Group, Deceuninck, Devan, Eco Treasures, ExxonMobil, Fraxinus, Gova, INEOS, Indinox, InOpSys, Janssen, Molecular Plasma Group, P&G, Port of Antwerp, Samsonite, Soudal, Tectero, and Total.

# Circularity and Resource Efficiency (CRE)

## What

The chemical and plastics industry has an important role to play in the realisation of a circular economy. In this innovation program, we innovate for the transformation of linear chemical value chains to circular value chains. Therefore, circular solutions are sought for all types of side and waste streams that arise in these chemical value chains. These include industrial side streams as well as post-industrial and post-consumer waste streams. In addition, the circular technologies that we develop can also help to increase circularity in other sectors.

In this program, we work on all side and waste streams that occur in the broad domain of the chemical industry, including for example used lubricants, paints or plant protection products and water. In addition to this broad scope, we have a strong focus on the circularity of plastics and the development of technologies for the recycling of plastic waste.

## Why

The main driver for this innovation program is resource efficiency. By making value chains more circular, dependency on virgin resources decreases. This way, our industry and society in general can deal with its limited resources in a smarter way.

Additional drivers are:

- increasing the value of side and waste streams;
- creating new value chains from side and waste streams;
- avoiding pollution.

## Goals

The goal of the Circularity and Resource Efficiency program is to, each year, develop a number of new processes that enable circularity by transforming waste and side streams into valuable products. This way, new value chains are created, starting from the waste or side streams over the conversion or recycling process up to the use of the resulting streams for the production of new products. By doing so, we want to underline the intrinsic value of waste and side streams and create value where before there was none. Our innovations will help to increase the recycling rate and circularity of waste and side streams as well as decrease the overall environmental impact of chemical and plastic value chains.

Every project within this program has the ambition to deliver an innovation in one or more phases of existing or new circular value chains, while safeguarding the valorisation potential of the whole value chain.

# Topics

## Plastics Sorting, Separation and Purification

### *What*

Sorting, separation and purification of plastic waste streams are critical steps towards increasing the recycling rate of both mechanical and chemical recycling. Depending on the recycling technique, the feedstock is often limited to polymer(s) of a certain purity. Improving these sorting, separation and purification technologies is therefore similarly important as innovation towards the recycling technologies themselves. The challenge is two-fold, both separating different polymer types from each other as well as removing additives, fillers or dyes, etc. from within the polymer itself is required.

### *Why*

The composition of the waste streams of polymer articles can vary from a stream composed solely of rigid bottles (mainly PET and PE) to streams containing additional trays, pots and films, with a wide range of different polymers. Rigid plastics can contain films which are often multi-layered, and hence difficult to separate. Bottles can be covered in PVC sleeve labels, or PET grade materials need to be separated from bottles and trays. Furthermore, applications polymers are often mixed with other materials (e.g. wood, metals, oil, etc.) and can contain legacy additives, such as brominated flame retardants (BrFR) and also organic additives such as plasticisers and dyes for which sorting and separation is difficult. To recycle these streams efficiently, the sorting of polymer articles by their constituent materials is of primary importance. This sorting ensures a minimum of waste and a high-quality and high-purity end-product. This sorting is particularly tedious for small or light plastic items due to their specific geometry, morphology, and low weight. The two main routes currently employed, namely wet and dry sorting, still require further technical enhancements and cost reduction to ensure a wide deployment and an increase in the overall recovery yield of plastics. Special attention should be given to both the construction and the packaging sector as well as to biobased polymers for which the current level of recycling is not as high as for fossil-based polymers due to the lower market volumes. Next to sorting, purification is another crucial step in obtaining circularity. An important technology for purification is dissolution or physical recycling. Physical recycling is the selective dissolution and subsequent recovery of the polymer(s) and potentially additives. The chemical structure of the polymers remains intact whilst additives can be removed in an efficient way. This allows for removal of e.g. unwanted substances/layers : additives, glues, metals, SVHC's … or remove odour or colour from plastic waste streams with the goal to increase quality and add value to the plastic waste stream.

### *State-of-play*

The proper identification of the materials is essential for achieving a maximised purity of recyclates. For this purpose, various technologies such as near infrared (NIR), laser, or x-ray-based techniques are available. NIR-units are widely used and form the state of the art in several European countries for sorting mixed post-consumer packaging. Although sorting technology has increased its accuracy, sorting efficiency never reaches 100% due to separation flaws and laminated or blended products that cannot be separated into their original materials. This often leads to contamination of recycled plastics with other plastics and all kinds of additives. The quality of sorting processes is also dependent on the efficiency of collection schemes, which vary widely even within EU member states.

For Flanders, the Catalisti ICON project MATTER focused on the expanded blue bag PMD+, to map the various plastic waste streams and identify their optimal recycling pathway. If the quality is sufficient after sorting and reprocessing, the recycled materials can be reused in the same or similar products. By recovering plastic materials for reuse, virgin plastic materials are replaced, contributing to a circular economy. However, insufficient sorting will result in a lower quality material, often only allowing the use in lower value applications (so-called down-cycling). Therefore, using solvents to purify plastic waste streams and further increase the quality of the plastic waste stream is becoming increasingly important, innovation in solvent systems and efficient solvent use will be necessary to improve the current mechanical recycling rate and facilitate the future chemical recycling rate. In the Catalisti project Remove2Reclaim, investigation in TiO2 removal from PS and PVC will be done via innovative solvent systems.

### *Next steps*

In the case of wet sorting, approaches like hydrocyclone and floatation still require further developments to strongly reduce their prohibitive cost (for hydrocyclone) and offer a better selectivity on light polymers and polymers having the same density (for floatation). Closed loop processes to eliminate contaminants, best sorting for higher quality batches together with selective precipitation should be considered.

In the case of dry sorting, improving polymer identification methods based on optical spectroscopies like Visible (VIS), Near Infrared (NIR) and RAMAN spectroscopies as well as Mid Infrared Thermography (MIR-T) and Laser-Induced Breakdown Spectroscopy (LIBS) could increase sorting technologies. Also increasing the detection capabilities of X-ray-based techniques like X-Ray transmission imaging (XRT) and Energy Dispersive X-ray fluorescence (XRF), exploring the potential of Terahertz spectroscopy and development of fast and low-cost detection techniques for tracers with coupling to enhanced sorting mechanisms (air valves, robotic handling) and integration of Artificial Intelligence (AI).

For dissolution or physical recycling, techniques to remove contaminants, and especially colour pigments or odours and other additives, should be developed. For example, the employment of smart solvent combinations to convert coloured polymers back to neat colourless materials. Dissolution technology in combination with chemical recycling is also looked at to tackle multilayer plastic materials, one of the most difficult to recycle plastic waste streams.

## Mechanical recycling of plastics

### *What*

Mechanical recycling is the process of recovering plastic solid waste for re-use in plastics manufacture via mechanical means. The basic polymer is not chemically altered during this process. Recycled polymers can be reprocessed into new plastics using well-established melt extrusion techniques, i.e. extrusion moulding, injection moulding, blow moulding, vacuum moulding or inflation moulding. Generally, mechanical recycling is restricted to thermoplastics (e.g. HDPE, LDPE, PPMA, PET) as thermosets cannot be remoulded by heat. The presence of a polymer dispersed in a matrix of a second polymer may dramatically change the properties of the latter and compromise its re-use. The main disadvantage of this kind of recycling is however the deterioration of product properties in every cycle. This is due to reduction of the resin molecular weight due to bond scissions caused by water or acidic impurities. The presence of additives added during the production or impurities during the lifetime of these polymers can cause additional challenges in the recycling.

### *Why*

In principle, all types of thermoplastics can be mechanically recycled with little or no quality impairment. However, multiple recycling loops will always result in degradation of the material with a loss of quality. It is currently the largest form of recycling in Europe, representing the majority of the recycled quantities. Waste streams that can easily provide clean plastic of a single type in large quantities are ideal for mechanical recycling and represent a win-win situation from an environmental and economic perspective: environmental benefits from substituting virgin material generally exceed the environmental burden from collection, sorting, transport and recycling operations, while the costs of such operations can be outweighed by potential revenues from selling recyclates on the market, if the quality of the recyclates is sufficient.

### *State-of-play*

Mechanical recycling is a well-known technique to address a variety of plastic waste streams and already implemented by many polymer processing or recycling companies. Different Catalisti initiatives, as PROFIT, Alfibond or PVCircular aim at further increasing recycling rates of respectively household waste plastics, PUR or PVC plastic waste streams by collaborating throughout the value chain and identifying new end-products for these post-industrial or post-consumer plastic waste streams. Additives to increase the quality of mechanical recycled polymer waste and allow higher recyclate content in new applications are also being developed within the Catalisti ICON project PoCoPAdd, which focuses on PVC.

### *Next steps*

Although mechanical recycling has been researched, developed and implemented by many polymer processing companies for many years, specific enhancements to this technology could further increase the recycling rate. These enhancements can be divided into process or extruder design or development of new additives. For example, reactive extrusion to modify polymers during the recycling process or new mixers based on extensional flow (specific reactor) to improve dispersion and distribution quality for a wide range of viscosity ratios and avoiding thermal degradation. For additives, the development of new compatibilizers or stable reagents for high temperature processing are interesting, to allow processing of cross-linked polymers.

## Chemical recycling of plastics

### *What*

Chemical recycling is a process which converts polymeric waste by changing its chemical structure to produce substances that are used as raw materials for the manufacturing of new products. Multiple technologies e.g. solvolysis/depolymerization, pyrolysis and gasification are all defined as chemical recycling. The technology selection depends on the polymer type of the waste feedstock, the level of purity and the desired end products.

Solvolysis is to break the polymer chain back in to building blocks in certain polar and semi polar solvents (e.g. water: alcohol; glycol). These are excellent reaction media for depolymerization of certain plastics. This process applied on plastic waste, can deliver substantial advantages by leading back to the initial building blocks (monomers), with relatively high yield and selectivity at relatively low temperatures. During the decomposition, a mixture of monomers, oligomers, solvents and residues is created. The addition of catalysts can improve the reaction metrics. Polymers to be processed by solvolysis are for example polyurethanes, PET, textile polyesters. Solvolysis can also be pre-treatment for separation in polymer waste streams due to its high chemical selectivity. For composites, depolymerization also allows the recovery of fibres and fillers. In addition, circularity-by-design is expected to facilitate plastic waste treatment by depolymerization.

Pyrolysis is conducted at high temperatures and in the absence of oxygen; it is particularly applicable to mixed polymer waste that is not suitable for mechanical recycling. During the thermal decomposition, complex product mixtures of variable composition are produced. The decomposition products, in the form of liquid oil or gases, are valuable as fuel or chemical building blocks. A mixture of unreacted carbon char and ash remain as a residual. Pyrolysis is possible with or without a catalyst. Pyrolysis of mass consumption plastics like PE or PP result in defined value products (such as waxes, oils). Catalytic pyrolysis seems a viable route to plastic waste recycling. Integrated Cascading Catalytic Pyrolysis (ICCP) maximises product value with high BTX and aromatics yields, while being energy positive (overall generates heat). Feed composition flexibility is high due to orientation on aromatics, i.e. mixed plastics can contain aromatics-based polymers.

Gasification, as a thermochemical conversion process, can be considered as a promising technology for the chemical valorisation of plastics waste. The conversion process takes place at high temperatures - preferably higher than 1000 °C - to produce tar-free synthesis gas consisting mainly of H2 and CO. Ash remains as a residual whereas the non-volatile carbon char that would remain from pyrolysis is converted into additional syngas. Partial oxidation of the feedstock provides the energy to reach the high temperatures. Therefore, oxygen is the preferred gasification agent. However, steam is also utilized to moderate temperatures in the process and to increase the yield of H2. Gasification has the potential to be applied where waste cannot be treated neither by mechanical recycling nor by pyrolysis. Temperatures below 1000°C can be used to recover olefins from polyolefin plastic waste.

### *Why*

The tremendous growth in waste generation all over the world has become one of the global challenges. Municipal waste including plastic waste presents the opportunity to become an alternative feedstock. In 2016, the EU used about 50 million t of plastics per year, of which 27 million t of waste was collected. From this waste only 31% was recycled, 42% was incinerated for energy and 27 % was still sent to landfill, leading to a loss of valuable resources. The novel processes described above are being developed to allow more diverse plastic waste streams to qualify for recycling and transform these waste streams back into chemicals, fuels and materials in contrast to waste incineration and landfill.

These advantages of chemical recycling compared to mechanical recycling will allow a rapid increase of the recycling rates and these waste valorisation processes will create new business opportunities for the recycling industry across Europe. They will also allow the reduction of the environmental footprint associated with the end of life of products in a wide range of sectors including consumer goods, packaging, textile, agriculture, transport, buildings, infrastructures. To obtain both ecological and economic benefits of these technologies, trade-offs towards higher amounts of energy and CAPEX costs will be required.

***State-of-play***

The waste-to-monomers through solvolysis or depolymerizations is relatively well developed for some types of polymers (TRL 3-5), for instance for polyethylene terephthalate (PET) and polystyrene (PS) but are lacking behind for polyolefins. Pyrolysis technologies are currently at TRL 3-5 with a range of maturities that go from concept-stage all the way to small demo plants depending if waste-to-fuel or waste-to-chemicals is considered. Within the Catalisti projects WATCH, MATTER and P2PC, pyrolysis techniques are investigated and are laying the foundation for a demo-plant. Gasification processes, which can possibly be combined with biological and chemical post-treatment, show a wide TRL range while currently different pilot and demo plants are under investigation.

***Next steps***

For solvolysis, ensuring a constant input of End-of-Life (EoL) material will be required to ensure the success of this technique together with a critical pre-treatment step of input material to ensure a level of purity. Increasing the robustness of the process to deal with the potentially high content of impurities of EoL materials should also be improved. Developing towards a continuous process instead of batch process could improve the competitiveness at commercial scale. After the solvolysis, downstream separation and purification of individual monomers will require further development. The large volumes of solvent used for this process will require significant amounts of energy for solvent recovery.

For pyrolysis, the prevention and/or removal of hazardous and corrosive compounds that can be generated during the process are critical, as they can affect the process complexity, scalability and safety. Avoidance of hetero-atoms and halogens in the input-stream by tailor made sorting technologies could address this issue and simultaneously increase the available input volume of polyolefin fraction for pyrolysis. Development towards reducing or avoiding reactor fouling due to by-products (cokes, ash) are also required. The development of catalytic pyrolysis to increase monomer recovery from solid plastic waste.

A specific challenge towards gasification is the efficient feeding system of waste material at high pressure gasification, in a continuous process together with the high temperature/energy requirements of the process itself. Also for this technique, attention should be given to avoid fouling due to by-products (ash and particles). Depending on the waste stream used as feedstock, tars, heavy metals, halogens and alkaline compounds can be released within the product gas, causing environmental and operational problems for the gasification, better separation of the feedstock to avoid the source of these pollutants is required, or the removal of the pollutants from the product gas is needed. Increasing the robustness and process flexibility to cope with short-term and/or long-term variation of waste feedstock composition could further increase the success of this technology.

## Valorisation of side streams from chemical industry

***What***

Side streams can be defined as end-products of various processing industries that have not been recycled or used for other purposes. These side streams can include liquid and solid streams such as used lubricants and paints but also gaseous streams such as waste heat or carbon monoxide. Biomass side streams are addressed in the program “Biobased Value Chains” and therefore not part of this program. Side streams coming from the plastic industry or water are addressed separately in CRE. These side streams can be valorised internal or external. The latter case is often referred to as Industrial Symbiosis (IS), which is defined as the use by one company or sector of underutilised resources broadly defined (including waste, by-products, residues, energy, water, logistics, capacity, expertise, equipment and materials) from another, with the result of keeping resources in productive use for longer.

### *Why*

Application of this concept allows materials to be used in a more sustainable way and contributes to the creation of a circular economy. The transition to such an economy will result in the increase of Europe's economic competitiveness, sustainability, resource efficiency and resource security. It also contributes to the reduction of greenhouse gas emissions.

Valorisation of side streams serves to reduce the environmental footprint of the industries involved. Virgin raw materials are required to a lesser degree, and the need for landfill waste disposal is reduced. It also allows value to be created from materials that would otherwise be discarded and so the materials remain economically valuable for longer than in traditional industrial systems. In particular, IS creates an interconnected network which strives to mimic the functioning of ecological systems, within which energy and materials cycle continually with no waste products produced.

### *State-of-play*

Valorising side streams for internal use is not straightforward. The "easy" side streams are often already valorised, the envisioned valorisation pathway is not economic feasible, the scale for implementation is too small, technologies for valorising the side streams are not mature enough. Furthermore, in particular related to IS, there is still much debate about how to make it successful and about the factors that affect its implementation, including technical and organizational aspects, regulatory issues, companies' and stakeholders' involvement, as well as economic feasibility. Networking and innovation are also recognized as crucial aspects. An example of IS is Smart Delta Resources, of which Steel2Chemicals is one project of symbiosis between DOW and ArcelorMittal.

In 2012, the Symbiose project was initiated with the support of essenscia and FISCH. An offline symbiose platform was created and although various opportunities were identified, only a few matches were successful. Often the technologies which would allow partners to work symbiotically need to first be developed or adapted to the symbiotic interaction (e.g. pre-treatment of waste streams to be used as raw materials, removal of contaminants and adaption of the processes to different composition raw materials). In the beginning of 2020, OVAM launched its online platform "SmartSymbiose", a meeting place between the demand for and supply of materials.

### *Next steps*

Innovation in terms of the development of supporting technologies and the use of new digital technologies like artificial intelligence in case of IS has been identified as a key aspect in defining the success of valorisation of side streams. Technologies should be designed, developed and optimized to ensure their usefulness in complex, cross-sectoral systems of industrial symbiosis. Examples include $CO_2$ capture, storage and reconditioning technologies, novel purification technologies, more efficient heat-recovery technologies, process technologies for the efficient production of flexible energy storage carriers. Mapping of potential industrial symbiosis streams (energy/materials) and activities should be based on a technical methodology to identify cross-sectorial symbiosis using data-analytics/decision-making support derived from 'sector blueprints' to overcome confidentiality issues for industrial data exchange and availability. Furthermore, facilitation is seen as one of the most important elements to foster the establishment of IS. Catalisti, as a catalysing body, is well placed to promote IS and drive its implementation with optimum speed.

## Closing the water loop

### *What*

Our planet runs on water and so do many industrial processes. However, clean fresh water is often not available where and when humans need it and in many parts of the world it is a scarce commodity. Main drivers for an increasing water stress are climate change and competing water demands from industrial, public and agricultural water users. So, reducing the water footprint, for instance through re-using process water, is an important issue in industrial water use. Process industries are facing increasing water stress, e.g. more than 40,000 million $m^3$ of wastewater is treated in EU every year, but only 964 million $m^3$ of this treated wastewater is reused. Another important challenge in water processing is reducing the emission of substances that may be harmful to the environment, as well as the recovery and reuse of valuable components from water. An integrated industrial water management, fostering recovery, as well as recycling and reuse of water, high-value products and energy, is the key approach to identify, realise and coordinate water efficiency measures in the process industry.

***Why***
Increasing independency from freshwater by water recycling and reuse can help decoupling growing production from using primary resources, improving the industrial production environmental footprint, whilst supporting production. In addition, by recovering valuable (or even toxic) components and by reusing them, incineration of huge amounts of wastewater from chemical/pharmaceutical components can be prevented. This may prevent high financial treatment costs, as well as detrimental environmental impacts.

***State-of-play***
Currently, the Catalisti project portfolio of water-related projects is relatively modest. One success case however was the start-up of the company InOpSys, which provides integrated, chemical-technological solutions for the valorisation of (aqueous) process (side) streams through flexible, modular and mobile units. The good results obtained in the Catalisti project 'Plant on a Truck (or POAT)' helped to build up a strong business case for the start-up. The SuMEMS project, i.e. 'Sustainable membrane technology-based solutions for solvent-rich wastewater treatment', aims at realising a breakthrough in this field by developing innovative, efficient and economic membrane-based technology solutions for the sustainable treatment of these very complex solvent-rich waste waters in a holistic approach. In the EcoTox project, a group of 15 chemical companies is joining forces to develop a methodology for the ecotoxicological assessment of effluents of industrial wastewater treatment plants in the chemical industry.

With the goal to realise a closed water loop in the chemical industry, we see four challenges to be worked on.

1. Process water needs to be reused and recycled better. This can be achieved for example by integrating water treatment technologies in process development and scale-up, by development of extraction and separation technologies and by valorisation of low temperature waste heat from wastewater.
2. The connection with water and (treated) wastewater streams from other industrial and non-industrial (e.g. public, agricultural) water users allows for a multiple, symbiotic use of water resources (e.g. municipal wastewater as a resource for industry or treated industrial wastewater for non-potable urban reuse).
3. Separated streams of used water (e.g. wastewater of specific processes, washing water from plant cleaning) can be treated effectively at the source using decentralized/smaller treatment systems. This enables on the one hand an immediate reuse of these water streams in the same process or in others with comparable requirements. On the other hand, this enables extraction and valorisation of components out of these streams, close to production.
4. In process industries, the close interaction between industrial production and integrated industrial water management continues with an increasing digital transformation. New water technologies also deploy advanced digital solutions for water in networks of sensors in domestic and industrial water distribution systems, capturing and using this new information to enable real-time management and quality control. Digital solutions also extend to water treatment and the multiple use of water.

***Next steps***
We will expand the Catalisti portfolio of water-related projects by setting up projects that contribute to the closing of the water loop. These should find solutions for reusing or recycling of process water, for extracting toxic or valuable components out of wastewater, or for realising water symbiosis between different players. Digital technologies can support here. One of the challenges will be to demonstrate that circular water principles can be translated into concrete business opportunities, and as such, convince companies that it is worthwhile to invest.

## Link with other Catalisti programs

Sorting and recycling technologies
→ link with ASP (circular by design)

Digitalisation as enabler for the circular economy
→ link with PIT

## Link with Moonshot Research Trajectories

Strong link with MOT2 Circularity of Carbon in Materials. Follow-up trajectories of successful MOT2 projects can fit in this program.

## Active companies

Companies active in projects within the CRE innovation program include, but are not limited to: Agfa, , Ajinomoto OmniChem, ArcelorMittal, Borealis, Chemours, ChemStream, Circular Organics, Copaco, DCM, Deceuninck, Eastman, Govaplast, Govi, Indaver, INEOS, InOpSys, Kemin, Lybover, MATCO, Moax, OWS, Proviron, Recticel, Unilin, and Van Heede.

# Advanced Sustainable Products (ASP)

## What

In this innovation program, we develop new innovative products that are advanced and sustainable. All product categories that are a part of the chemical value chain are covered. We develop consumer products like paints, glues, plant protection products, detergents and cosmetics, but also intermediates that are further processed by companies more downstream in the value chain like plastic packaging, building materials, materials for the transport or energy sectors, and so on.

The focus in this program is on the functionality of the product in its application. Desired functionalities can be as diverse as lightweight for materials in the transport sector, flame-retarding for textiles and building materials, or better recyclable for plastic packaging. In any case, the new product, new functionality or new application will always be more sustainable than its predecessor. Innovation for substitution of substances of concern also forms an important part of this program.

## Why

The drivers for the development of advanced sustainable products can come from customer demand or from legislation. Customers, both end consumers and B2B customers, demand improved or new functionalities for their products. Also, the development of new applications can create added value in existing or new value chains.

The product regulation REACH forms an important framework for driving innovation towards products that have a lower impact on human health or on the environment. In addition, the push towards a circular economy is a driver for developing products that better suit circular value chains.

## Goals

The goal of the Advanced Sustainable Products program is to, each year, develop a number of new products for which it can be shown that they:

- have an improved functionality combined with a similar sustainability profile, or an equal functionality combined with a better sustainability profile;
- have an improved processability;
- enable a new sustainable application;
- contribute to safer chemical value chains;
- contribute to more circular value chains.

These new products will help our member companies to improve or enlarge their product portfolios, and as such acquire unique and strong positions in the chemical value chains of the future.

Every project within this program has the ambition to deliver such a product innovation.

# Topics

## Sustainable design: function and application

### *What*

This topic focuses on functionalities related to the use phase of a product. This can be a new, improved or additional compatible functionality, each time with a positive impact on the sustainability of the product.

### *Why*

The sustainable nature of a product is not exclusively determined by its design, raw materials and processing techniques for the production, or by the processability at their end-of-life. Also the usability of a product can highly contribute to the sustainable nature of a product. Within the topic sustainable design, function and application, we focus on functionalities leading to a higher sustainable character. This can be achieved by improving existing functionalities (higher quality, increased efficiency, improved barrier- or adhesion properties, etc...), or by developing new functionalities (self-healing properties, anti-bacterial properties, anti-corrosion properties, traceability, etc). In addition, it may be feasible to integrate products with specific functionalities within one new, more efficient, and thus more sustainable product.

### *State-of-play*

Examples of improved functionality are numerous and very broad. Potentially, prior knowledge is already available and thus concerns developments at higher TRL levels. However, sustainable-driven changes in chemical composition may lead to different behaviour. More fundamental research is then required to maintain equal properties despite disruptive compositional changes. An example are water-based paints which are ecologically and health-friendlier than their solvent-based variants. However, more frequent reapplication may be required, which substantially impacts the sustainable nature of water-based alternatives. Moreover, due to their lower quality, they are not yet accepted as a full alternative for critical applications. An example of compatible functionalities which are promising for synergetic integration is the CSP+ project. This Flux50-Catalisti intercluster project aims to combine 2 solar technologies to produce heat (CSP) and electricity (PV) using the same surface area to capture even more energy from the sun. It focusses on research on the design of solar cells, development of new transmission coatings and innovative integration technology to maximize the energy yield and thus minimize the Levelized Cost Of Energy of CSP systems, which will make the use of CSP systems economically more viable in regions, like Flanders, with a lot of diffuse light.

### *Next steps*

Catalisti will continue working on rethinking products paying equal attention to their functionality as well as their sustainable character.

## Sustainable design: feedstock and process

### *What*

Sustainable product design for feedstock and process is the concept to rethink the design of products by using alternative (sustainable) feedstocks or process technologies. So, there is no focus on the development of new process technologies or new feedstock value chains as such. Therefore, we refer to the programs PIT and BVC.

In this program, we want to improve the production efficiency in terms of limiting resource/energy consumption and waste generation, but also in terms of increasing the efficiency of the production process itself (for example by reducing the lead time with a maximum product quality). The production efficiency is seen as an important element of the sustainability of the product. In some cases, it can be necessary to completely rethink the way the product is manufactured by using different technologies and feedstocks.

### *Why*

Optimise the process of production to reduce energy and other resources and waste generation is very important. Feedstock choices and the production process itself have impact on many different parts of the product's life cycle and can possibly affect many different environmental aspects.

Therefore, it is important to support research that takes into account the whole value chain of a product in order to determine the most sustainable option in product development and design.

### *State-of-play*

To become more sustainable the chemical industry must reduce its dependence on petroleum and gas feedstock and shift to alternative, more sustainable feedstock. Europe has defined a set of Critical Raw Materials (CRW) to which it has vulnerable access. Innovative solutions need to be provided to reduce the dependency of this CRW through efficient and environmentally friendly recycling, the use of sustainable substitutions for the feedstock or simply reducing the amount of feedstock used.

One of the previous Catalisti projects, which is a good example of sustainable product design for process, focused on the development of a versatile and industry competitive method for the manufacturing of hybrid injection moulds using additive manufacturing technology (HYBRID MOULDS). The main output will result in a production method that combines reduced lead times and high quality (comparable with the classic production method) output of the final injection moulded parts. In this project, one of the big challenges is to produce inserts by additive manufacturing that are suitable for the use in hybrid moulds. This means to find the right print technique, to find the right print material, to search for the right algorithm to generate a print file that creates inserts who can deliver as close as possible the same results as metal inserts and finally to search for the best printing settings. Thus, the process of additive manufacturing needs to be optimised for the injection moulding application. Also, the quality of the AM products needs to be optimised. Quality parameters for the products made by additive manufacturing are heat, pressure and wearing resistive, shape retaining and low adhesion with the used injection moulding materials.

### *Next steps*

This program has a strong link and even overlap with the Biobased Value Chains and Circularity and Resource Efficiency programs for the feedstock aspect and with the Process Intensification and Transformation program for the process aspect. Nevertheless, we also include this topic in the Advanced Sustainable Products program to bring in focus on the product design and product life aspect. To optimise the product design in terms of feedstock and process, Catalisti will continue to work on this topic.

## Circular by design

### *What*

Circular By Design is the concept of integrating circularity of products when designing them. This can be done by "design for recycling" as well as by "design from recycling" In "design for recycling", products are designed to be easily recyclable or reusable. can include rethinking material choice, but also the product itself. In the case of easily reusable, we can speak of "design for reuse". In "design from recycling", waste streams or recycled streams are used as a feedstock for the production of new products. Here, the issue will be to deal with the characteristics of this alternative feedstock.

Another possibility to make plastics value chains circular, is to design biodegradable plastics. If plastics can degrade in their environment or in a composting installation at the end of their use phase, we can speak about a circular value chain. Such a circular value chain can be beneficial for some streams, for example mixed streams with organic waste, or for products that have a high chance of ending up in the environment.

### *Why*

The aim of Circular By Design is to reduce the generation of waste as well as the dependence on the extraction and use of virgin raw materials, and in this way, contribute to the realization of a circular economy.

The recycling rates for different material streams as well as the use of recycled materials is steadily growing. Despite this, only a small fraction of feedstock in our industry comes from recycled products and recovered materials. The use of a higher content of recycled materials in various products is an important step towards a sustainable supply of raw materials and the realisation of a circular economy.

### *State-of-play*

As producers and processors of plastics, our sector has a crucial role in the realisation of a circular value chain for plastics. A major challenge is the diversity of plastic, with a multiplicity of polymers, combinations and applications. This diversity results in complex plastic waste streams, for which sorting and recycling technologies need to be developed and implemented. In addition, we should think about designing products in function of recyclability and of designing products based on recycled streams.

From the very start of the design process, recyclability should be included and the product design should in any case be aligned with the layout of the waste handling and plastic waste sorting. Compatibility of materials, easy separation, the use of additives, … play a role in determining the recyclability of a given product. Also, the use of recycled content in new products should be investigated.

One of the previous Catalisti projects focused on developing technologies to separate different layers found in complex materials in such a way that maximum separation is made possible (RECYCOAT). Another ongoing Catalisti project has the aim to design additives to boost post-consumer PVC up to a level of virgin PVC and in turn increase the amount of post-consumer PVC recyclate content in current and new products (PoCoPAdd). Also, in the topic design for recycling Catalisti has gained expertise, i.e. reverse engineering products with recycled content and define and produce feedstock from recycling which are fit for use (PROFIT).

### *Next steps*

In order to achieve circularity, this topic is an important complement to the program Circularity and Resource Efficiency, as it is necessary to supplement the research on the recycling process itself with the research on the design of products in function of recyclability.

The success of a circular plastics economy will depend on the ability of plastic recycling and the quality of the reused plastic, which is nowadays often poor and therefor has very limited usability. Therefore, Catalisti will continue working on the design of products to increase the recyclability of used products (design for recycling) and to elevate the use of high-quality recycled content in new products (design from recycling).

## Safe by design

### *What*

Safe by design is an approach to rethink products and processes to minimize, and preferably eliminate, harmful effects on health and environment throughout the life cycle. Yet, safety aspects are preferably considered early in the innovation process when crucial choices are being made about raw materials, processes, basic techniques and applications. Therefore, this topic highly relates to innovation programs BVC, PIT and CRE. Substitution of hazardous compounds may imply the use of biobased feedstock, alternative process and production technologies allowing the use of more safe components, as well as the elimination of legacy additives which may cause phase-out of hazardous compounds, among others during recycling processes. In this way, companies prevent problems that may arise later. The safe by design topic within ASP focuses on the substitution of (potentially) hazardous compounds on molecular, material and product level.

### *Why*

The transition to a safe and circular chemistry offers unique opportunities for Flanders, and by extension Europe, to create economic added value through innovation with products and processes that are safer, cleaner and more energy efficient. Regulation, in particular REACH, inevitably has an impact on the degree of innovation, replacement and substitution activities. However, it is important that these innovation activities are not only policy-driven, but also lead to increased quality and thus competitiveness.

***State-of-play***
Most products containing hazardous compounds have a well-proven effectiveness and are therefore being used for decades. Typically, these products have been developed using a trial-and-error-based methodology, meaning that the mechanisms that lead to these desired technical properties are not always well-understood. Evidently, this complicates the quest for safer alternatives. Additionally, when safer alternatives have been identified, they might not meet the technical performance compared to traditional hazardous products, which implies that they cannot be used in critical applications. Finally, when safer alternatives have been identified with equal or even improved performance compared to traditional products, undesired side-effects can appear. In that case, additional components are added to counter these undesired side-effects. Consequently, safe by design is rarely a 1 by 1 substitution but requires complete rethinking of products.

Previous Catalisti projects related to the reformulation of products containing (potentially) hazardous chemicals include substitution of SVHC listed chemical foaming agents (FREEFOAMING), halogenated flame retardants (PolyFlam) and debatable surface treatments (PlasmaSol). In the debate of reducing VOC's, one typically looks into biobased sources as alternative for petroleum-based products (AMBER, BIORESAL, MAIA). However, shifting from solvent- to water-based products is still challenging with respect to the functionality of the end-product. Increased research on how to meet technical challenges using clean and safe resources could lead to valuable business cases.

***Next steps***
We will continue to support research and innovation for safer alternatives of potentially harmful compounds and products. The development of safe alternatives occurs in 3 major steps; (1) Detection: as regulations and societal concerns continuously evolve, continuous research is required to identify safer alternatives for different types of compounds and products. (2) Technical performance: safe alternatives rarely meet the technical properties of conventional (potentially) harmful products. Increased research on how to meet technical challenges using clean and safe resources is needed. (3) Long term risk and life cycle assessment: next to finding safe alternatives with similar or improved technical characteristics, it is also of high importance to perform risk assessments and to consider the long-term performance of newly developed products. Therefore, also research on human and eco-toxicology and environmental behaviour fits within safe by design.

## Link with other Catalisti programs

Sustainable by design: feedstock and process
→ link with CRE, BVC, PIT

Circular by design
→ link with CRE

Biodegradability as a new functionality
→ link with BVC

Safe by design
→ link with BVC, CRE, PIT

## Link with Moonshot Research Trajectories

There is no direct link between the ASP Program and the MOTs. As the Moonshot program is mainly focused on breakthrough technologies in processes and value chains, the product focus of the ASP program is not explicitly present. However, for one topic, circular by design, there is a link with MOT2 Circularity of Carbon in Materials.

## Active companies

Companies active in projects within the ASP innovation program include, but are not limited to: Agfa, Azteq, B4Plastics, Balta, Beaulieu, Borealis, Concordia Textiles, Deceuninck, Engie Laborelec, I-Coats, Kaneka, Lawter, Matthys Group, Nyobe, Oleon, Plastibert, Recticel, Samsonite, Sioen, Soltech, Vetex, and Zigg Zagg.

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