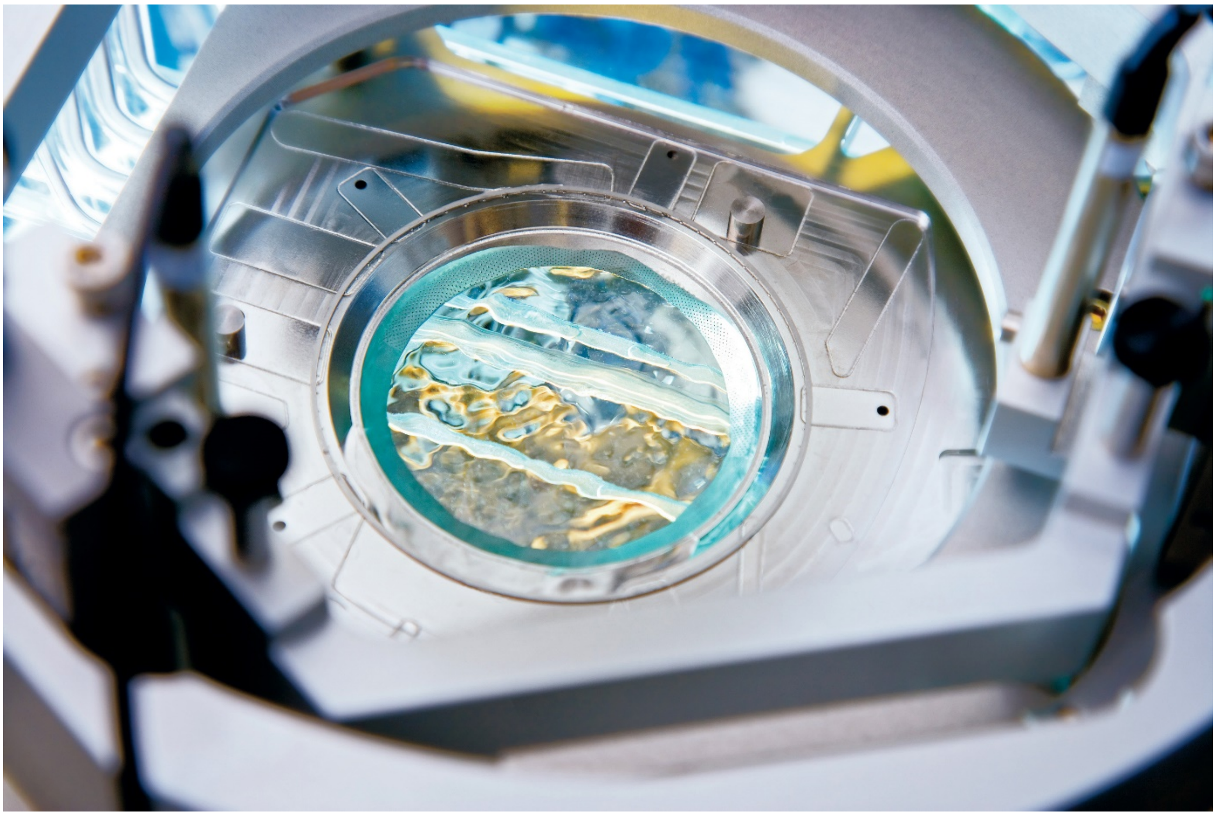
Roadmap
Chemical Conversion, Process Technology & Synthesis



Roadmap Chemical Conversion, Process Technology & Synthesis

Making sustainable chemical products

Innovative chemistry for sustainable growth

Number one on the list of Global Challenges we find the need for sustainable development and the necessity to address the climate change. High on the list as well is the Global Challenge to sustainably meet the growing energy demand. The field of chemistry is ready to take on a key role in helping to tackle these challenges. At the same time, it will have to deal with the changes these global developments will impose on the sources of raw materials and energy which have been the basis for the chemical industries for many decades. In particular, catalysis, process technology and synthesis are crucial disciplines when it comes to establishing the scientific and technological foundation for making cleaner, more efficient, economically viable chemical production processes, and enabling a change in feedstock and energy sources to fuel our processes.

In this document, the program council describes how circularity and the use of bio-based feedstocks will play a more and more important role. It addresses how it will use catalysis and process technology for the production of functional molecules, materials and (precursors for) energy carriers, making use of the current and future feedstocks and energy sources. With the strongholds for these fields of expertise in the Netherlands, it is indicated how reactions, catalyst materials, reactors, and production processes shall be integrated at all length- and time scales of importance. These aspects jointly will be instrumental in retaining the competitive edge of chemical industry and catalyst industry in the Netherlands (2023). The overarching ambition for the year 2040 is to complete the transition from our fossil resource dependent economy to a circular low-carbon economy that relies on sustainable and abundant resources. A roadmap is presented that includes chemical technologies to realize this ambitious goal.

1 Introduction

This roadmap combines the fields of catalysis, process technology and synthesis of functional molecules. The integration of the four subjects has led to a coherent view in which three main tasks are defined:

- *Making Molecules Efficiently*, where themes s.a. C_1/N_1 chemistry, CO_2 utilization, process efficiency are found, and where the competencies within catalysis and process technology are addressed.
- *Making Molecules circularly*, which includes recycling and design for circularity.
- *Making Molecules from biomass,* which focuses on the specific challenges encountered in using bio renewable feedstock.
- *Making Functional Molecules*, dealing with high performance materials, and the important synthesis competency in specialty, pharma and fine chemicals.

The roadmap targets multi-scale understanding all the way from active sites (nm), particle agglomerates (μm) to catalyst particles (mm), to reactors (m) and the refineries or chemical plants in which they are integrated, as well as the time-scales governing chemical reactions (ps) via transport phenomena (ms) to the complete lifetime of a catalyst (minutes to years).
Catalysis, Process Technology and Synthesis are the central sciences in designing more efficient and cleaner routes to new functional materials, producing less (ultimately: zero) waste, reducing CO_2 emissions or even utilizing it.

The Dutch economy and its chemical industry are highly intertwined with the European chemical industry. The European commission has defined Mission areas and global challenges for the next decades in its **Horizon Europe** framework program. Chemistry, and in particular also catalysis, process technology and synthesis will play an important role in fulfilling these missions and challenges. The same is true for the Meerjarige Missiegedreven Innovatie Programma's (MMIP) that have been defined in the Netherlands. This roadmap therefore not only described a vision as formulated by -representatives of- the various fields within Chemical Conversions Process Technology & Synthesis, it also addressed the overlap with the MMIP's.

KIA	**MMIP / Mission**	Making molecules efficiently	Making molecules circularly	Making molecules from biomass	Making functional molecules
Energy transition	6: Closing industrial cycles	x	x	x	
and sustainability	7: CO2-free industrial heat system	x			
	8: Electrification and radically new processes	x			
	13: A robust and socially supported energy system	x			
Agriculture	A: Circular agriculture			x	
Key Technologies	1: Chemical technologies	x	x	x	x
	7: Life science technologies			x	

1.1 Why should we do this?

The research directions proposed in this document relate to the Missions as described in the Knowledge and Innovation Agenda. It will contribute to more efficient use of resources, resource recycling, reduction of waste and pollution, and conversion of waste to useful raw materials. It will create higher educated jobs, and promote resource independence, as well as novel sustainable routes to biomedical, food, feed, fertilizers and speciality products. It will lead to increasing use of progressively lower cost sustainable resources, and improve European competitiveness towards Asia, USA, and the Middle East.

1.2 Why should we do this in the Netherlands?

The Chemical industry generates approximately 60 billion euro in revenues, and contributes about 23 billion euros to the trade balance (or 52% of the total). About 57,000 people are employed in the chemical industry. The annual budget for R&D in the Dutch chemical industry is approximately 900 million Euros. About 85% of all chemicals are made through catalytic processes. Since the Netherlands combines a concentration of catalysts and enzyme producers, catalyst and fermentation users, and world-class academic research groups, (bio)catalysis, organic synthesis and process engineering and downstream processing are strongholds. Industrial players are closely involved in academic research, and actively participate in public-private-partnerships. Synthesis of functional materials (e.g. bioactives developed in SME's), and polymeric materials (through homogeneous or heterogeneous catalysis or fermentation), is another strong point. In addition, the infrastructure in the Netherlands is ideally suited for the realization of a circular economy. The infrastructure in the ARRRA (Antwerp-Rotterdam-Rhine-Ruhr-Area) cluster is well equipped to handle large amounts of biomass (wood and straw type). The agricultural knowledge will provide very high production yield crops (e.g. 15 ton sugar per acre). The combination of sea ports, green energy supplying providers and big refineries give the energy integration required for successful biorefineries.

2. Overview of tasks

2.1 Making molecules efficiently

In 2040 the majority of chemicals are no longer synthesized with the use of fossil fuels. Chemists and chemical engineers are striving for this mission, which is aligned with mission C in the knowledge and innovation agenda on the energy transition and sustainability. It is not trivial to get to this point and much of the research of today has to be implemented in an industrial setting.

One great step in adopting processes with greater energy efficiency is the use of small molecules as building blocks. Innovations relating to the use of molecules like CO_2, water and nitrogen can be used to close industrial cycles, described in MMIP 6 and MMIP 13. Here CO_2 can be used as a carbon source, water as a hydrogen source and nitrogen can be used in making ammonia. In addition to improving traditional heterogeneous catalysts, radically new processes can be used to achieve this, as described in MMIP 8. These processes can utilize electrical energy, sunlight or a combination of the two directly for chemical conversion. The chemical key technologies ST1-3 and ST1-4 on catalysis and electrification contribute to this.

Adopting these new processes brings challenges for the chemical industry. One important factor is the use of heat, described in MMIP 7. Efficient use of heat, optimized reactor design, process systems engineering and separation technology all play a role in the transition to new sustainable production of chemicals. The development of chemical key technologies ST 1-1 and 1-6 on process technology and separation technology are relevant here.

The discipline of Process Technology (PT) will play an important role in the upcoming transition towards sustainable chemical, refinery, food/feed and energy industries. Being able to develop and implement technology at world-scale without (all) the fundamentals being known is a key strength of Process Technology and a necessity to reach the 2050 goals. In 2050, sustainable feedstock and energy sources will be used in the industry and new products with improved functionality and recyclability will be manufactured. History has shown that, in peace time, it takes often 30 year for a new technology to grow from existing (TRL-9) to taking 1% of the market [Kramer & Haigh, Nature]. This time constant does not even come close to what is needed to reach the sustainability ambitions of 2050. By means of its integrated and system level approach, Process Technology will take the lead in scaling up the new technologies required and will do this with unpresented pace in order to meet the 2030 and 2050 goals. This will require:

1) Close collaboration of PT with disciplines like chemistry, catalysis, materials science, automation, etc. in parallel development trajectories.
2) Making use, wherever possible, of existing knowledge, materials and infrastructure, while also exploiting novel possibilities for process intensification, electrification of the chemical industry, better control and optimization via artificial intelligence, etc.
3) Better and faster design and scale-up methods. This could include: i) quick scan methods to identify opportunities and, even more importantly, show-stoppers, ii) fast screening experimentation, iii) design / scale-up in silico, etc..
4) Making processes economically viable at capacities an order of magnitude lower than practiced in the fossil era due to distributed availability of renewable resources.
5) Connections, more and different than now, between the refinery, chemistry, food/feed, and energy sectors. [As an example: it might be worthwhile to consider feeding some waste plastics as reducing agent to the steel industry and re-use the CO in the offgas instead of chemically recycling these plastics].

Process Technology will contribute to (amongst others):

- Energy savings. Many processes, mostly separations, are still operated far from the thermodynamic minimum leaving room for optimization of existing processes and new concepts such as non-heat driven separation.
- In the transition period, development and optimization of “as clean as possible” fossil-based processes. C_1-chemistry is an example, e.g. methane pyrolysis coupled to carbon sequestration.
- Introduction of sustainable energy sources in the industry. Examples are electrical heating, heat networks, and electricity-based reactions and separations.
- Improved circularity of processes and products. Not only carbon-based products should be addressed, but also scarce metals required for energy storage & catalysts and food related atoms such as P, N, K must be considered.

- Introduction and efficient use of renewable feedstock. Here the focus will be on carbon. As we cannot recycle jet fuel and 100% recycling of materials is not possible, the future requires processes that take-in recyclate and renewable C-sources such as biomass and CO_2
- Development of technology to store energy. Particularly this technology and electrolysis will benefit from a shift from materials science dominance to scale-up (PT) in order to reduce the costs significantly.

Expected results present – 2040

Scientific/technological goal:

- Novel processes based on natural gas (methane, ethane), biomass, and especially CO_2; novel (bio)catalysts and processes for the direct conversion of methane into reactive intermediates compatible with current chemical industry. Novel (bio)catalysts and processes for syngas conversion into a broader range of products than only fuels (olefins, alcohols); also direct Fischer-Tropsch conversion to fuels (optimization current catalysts, catalyst stability, feedstock flexibility, improved product selectivity). Novel (bio)catalytic processes for methanol conversion into olefins, gasoline, and diesel. Integrated (bio)catalyst/reactor technology research to increase development of novel (bio)chemical processes (decrease time from discovery to market). Efficient technologies for energy transfer to processes with a high energy demand (e.g. dry reforming). Efficient purification/separation of mixtures of hydrocarbons from each other by other means than the existing technologies (e.g. membranes and sorption technology).
- Inclusion of processes based on the technologies summarized above in the process mix.

Industrial end goal:

- Climate-neutral chemical industry while being economical with critical raw materials, flexibility in operations: being able to deal with fluctuating electricity supply.

Societal goal:

- Realization that transition to fossil-free economy will be time-consuming and takes large efforts.

Suitable funding frameworks:

- Large-scale programs that combine close industry/academia interactions (CHIPP-type) with broad (TA-type) consortia to address fundamental chemistry/engineering aspects of novel conversion technology.

Milestones:

- New (bio)catalytic processes CO_2 conversion to platform molecules (2025); low-energy separation processes for hydrocarbons mixtures (2025).
- Inclusion of new, renewable catalytic processes for production of H_2 and conversion of CO_2 to platform molecules (2025); low-energy separation processes for hydrocarbons mixtures (2025).

2.2 Making molecules circularly

Traditional linear value chains lead to a take-make-dispose mindset and leads to waste. Reduction and recovery of that waste is important for closing industrial cycles, as described in MMIP 6. This starts in the design of chemical products; when taking recycling explicitly into account, waste streams can be treated much more easily. After separation of waste streams, enabled by the chemical key technology ST1-2 on analytical chemistry, chemical recycling is the preferred route to creating renewable feedstock. Doing so will not only decrease CO_2 emissions and pollution, it will also safeguard the availability of critical elements that are needed in many high-tech applications. Plastics are still being incinerated for energy recovery and chemical recycling approaches will provide a solution for closing the carbon cycle. Just like plastics, emission of phosphorus and nitrogen into the environment also causes pollution. The effect on the recovery of such elements will contribute to mission A on sustainability, set in the agricultural innovation agenda. In addition to these elements, many more critical elements are incorporated in materials that are currently not being recycled.

Expected results present – 2040

Scientific/technological goal:

- Energy efficient chemical conversion of waste streams.

Industrial end goal:

- Circular industry of critical elements with a well-established supply chain.
- Use of 50% renewable resources / essential elements by the chemical industry in 2030/2040..

Societal goal:

- Closed biochemical element cycles and no pollution of essential elements into the environment.

Suitable funding frameworks:

- Programmes that can strengthen research groups working on the topics of chemical recycling of critical elements and combine close industry/academia interactions.

Milestones:

- Promoting the use of renewable sources for critical elements and developing the needed circular technologies in order to do so.

2.3 Making molecules from biomass

Apart from using small molecules mentioned earlier, larger molecules present in biomass can also be used as feedstock. The five main classes of compounds in the biomass that can be used are cellulose, hemicellulose, lignin, lipids, and proteins. These molecules contain energy that can be utilized but are also highly functionalized. The use of bio-based feedstock to close industrial cycles is described in MMIP 6. It also has overlap with the innovation agenda of agriculture in mission A. Biomass has multiple uses and must be used diligently to avoid competition with food. The commercial valorization of biomass to fuel, chemicals, and materials has been narrowly limited to a few value chains, and broad commercialization has yet to be realized.

Various techniques need to be developed further to use biomass as feedstock. The chemical key technologies ST1-1, ST1-6, ST7-1 and ST7-6 on bioprocess and separation technology and biocatalysis and biotechnology contribute to this. Separation is needed due to the highly heterogeneous nature of biomass makes separation an important factor. Technologies like pyrolysis, biocatalysis and biotechnology are important for the use of biomass. This would provide new routes for making fuels and chemicals in a truly sustainable way. Gaining a detailed understanding of (bio-)catalysis, process technology, agriculture, and biomass production chains and downstream processing is therefore essential.

Expected results present - 2040

Scientific/technological goal:

- The goal is to further strengthen the worldwide prominent position of Dutch (Bio-)Catalysis and process technology R&D of biomass conversions.
- Efficient purification/separation (e.g. water and salt removal) of bio-origin molecule mixtures based on other separation principles than boiling point difference with minimal energy input.
- Developments in process intensification. e.g. by development of better biocatalysts, bioreactors and downstream process technology. Real integration/optimization between the industrial biotechnology and chemical catalytic conversions, e.g. biomimetic catalyst, enzymes working under even more extreme conditions (e.g. non-aqueous solvents, high T, high P).
- Zero waste, including recycling and conversion of e.g. CO_2 side streams.
- Insight in the relation between bio-based feedstock specifications, bio-refining and product specifications

Industrial end goal:

- To produce significant amounts of chemicals produced in the Netherlands from a biobased origin, with maximum CO_2 reduction (Commissie Corbey).
- Introduction of demo and commercial scale biorefineries will attract additional conversion and processing activities down the value chain and the resulting learnings will create a new innovative climate (Bioport instead of Silicon Valley).
- Development of process intensification and integration will further lead to an overall growing efficiency and will boost the cost competitiveness of the Dutch biobased economy. Closure of water, nutrients and mineral cycles around bio-refineries/biochemical production.

Societal goal:

- General acceptance that the use of biomass as feedstock for fuels and chemicals is desirable. To achieve this goal all important socio-economic aspects and sustainability issues need to be identified, and adequate systems to monitor and model these parameters should be developed. In addition, one should aim at the development of respected education, communication and valorization programs.

Suitable funding frameworks:

- National and Provincial governments, NWO, EU (Horizon Europe, PPP Biobased Industries Consortium (BIC) and successors).

Specific steps required present - 2040

Short term

- Implement demo- and flagship-scale biorefineries in the Netherlands. Facilitate the production of fractionated second generation sugars under world market price of sugar/dextrose to attract interest from producers of first generation products like lactic acid, succinic acid, enzymes & antibiotics, FDCA and furfural. Develop novel processes and products based on industrial biotechnology and chemical catalysis.

Medium term

- By using novel biocatalysts, process intensification type of R&D novel processes are developed up to 2030 in order to be implemented from 2030 to 2040. Selection of novel products will be based on carbon (molecular formula should not differ too much from the C-H_2-O composition of C_5/C_6 sugars) as well as electron efficiency to optimize/maintain atom efficient conversions/products; integration of different types of fermentation (to improve carbon cycling) is desirable.
- Selection of novel process will be based on drivers of ecology and economy;
- Increased emphasis on nitrogen-containing molecules, such as those derived from amino acids.
- Increased emphasis on the production of biopolymers and food/feed replacements/additives.

Long term

- Scaling up biorefinery clusters including energy integration, energy use of other sustainable clusters.

2.4 Making functional molecules

Synthetic chemistry is a key enabling science for the design, synthesis, and modification of functional molecules, which are part of speciality chemicals such as pharmaceuticals, hormones, vitamins, pesticides, personal-care products, and fine chemicals. While these functional molecules are typically relatively small molecules with complex structures, polymeric functional molecules form a wholly different class, and make up materials widely used in the production of textiles, paints, cleaning agents, tires, insulating materials, packaging, for biomedical materials, regenerative medicine. Thus, functional molecules play a vital role in our daily lives and are of high relevance for the pharma, agro, health & food, transport and energy sectors.

Specialty, pharma and fine chemicals demand, strong synthesis and catalysis capabilities. However, currently access to funding for technology development or improvement in synthesis and/or catalysis is circumstantial as synthesis and catalysis are seen as enabling elements for new(MMIP-driven) projects, rather than as driving themes per sé.

Expected results present - 2040

Scientific/technological goal

- Exploit, instead of removing) the functionality present in biobased and/or molecules derived from chemical recycling towards high performance materials.
- Toolbox of synthetic methods available for the synthesis of complex functional small molecules and catalyst design tools to allow specific 'on demand' activity/selectivity;
- A toolbox of modular equipment, technologies and sensors enabling the implementation of multi-purpose flexible production systems with reaction, separation and if necessary formulation. The ability to produce functionality on demand (in time and place) by a comprehensive understanding of the relation between process/equipment, molecule and functionality.
- AI/ML methodologies for synthesis route planning and process design and optimization widely available and used.

Industrial end goal

- Fully integrate waste and biobased streams in the monomer selection step for chemical product design.
- Sustainable and robust manufacturing of any required end product through catalytic processes using abundant and renewable raw materials;
- A leading position of the Netherlands and Europe in the production and supply of fine and specialty chemical molecules/products.

Societal goal

- Show the relevance of biobased and recycled streams for high performance materials and showcase concrete examples of this approach
- Cost-effective end products with lower environmental impact of chemical manufacturing;
- Conservation and creation of knowledge-intensive jobs in the fields of the production of functionality and production systems;
- Intrinsically safe and resource and energy efficient production of fine and specialty chemical molecules/products.
- Security of supply dilemmas of key complex chemicals de-risked.

Specific steps required present - 2040

Short term

- Synthetic methodologies and catalysts must continuously evolve and improve thereby expanding the range of complex molecules available via sustainable (catalytic) synthesis. catalysts based on abundant metals and cheap ligands as well as metal-free catalysts have to be developed. To evaluate the newly developed synthetic methodologies and catalytic systems relevant sustainability metrics must be applied. LCA (Life Cycle Analysis) tools to judge specialty chemical products and processes is routinely available and easy to use.
- Reduction of the costs of modular reactors by the introduction of advanced production technologies . Development of modular separation technologies.

3. Principal activities of tasks

3.1 Making molecules efficiently

The need to make molecules more efficiently is addressed in this paragraph from two angles. From one angle themes are described related to feedstock diversification which will be of great importance to create a low carbon foodprint chemical industry. This deals with C_1 chemistry using methane or CO_2, as well as with the use of sustainable resources s.a. electricity and light. From the other angle the competencies catalysis and process technology are described, since the progress on the themes will heavily depend on these competencies.

3.1.1 Feedstock diversification: C_1/N_1 chemistry

The focus of the chemical industry is to become climate neutral by 2050. This will require the development of climate-neutral and circular-economy solutions by the industry; the Netherlands can become a global leader for developing such technologies.
To be able to generate (nitrogen containing) carbohydrates, an alternative renewable basis of production could be to use the resources CO_2, H_2O, and N_2. For the generation of chemical building blocks, a few reactions from these three resources appear particularly interesting, also with the view on environmental impact.

- $CO_2 + H_2O \rightarrow (CO + H_2) + O_2$ (1)

Reaction (1) aims at the production of syngas (a mixture of CO and H_2), which is now typically produced by the so-called methane-steam reaction:

- $CH_4 + H_2O \leftrightarrow CO + 3\,H_2$ (2)

The disadvantage of reaction (2), is that the endothermicity of the reaction requires very high reaction temperatures, which are typically generated by burning of additional methane, leading to significant emissions of CO_2. In principle, (renewable) electrical heating can be used to drive the endothermic reaction, which would make steam reforming more environmentally benign.
For the long term, CO_2 should become an important carbon source for the chemical industry, either in concentrated form from industrial processes or from direct air capture. Three main routes for CO_2 conversion are feasible. First, the indirect route: CO_2 is converted with sustainably produced hydrogen into syngas, which can be used in "traditional" chemical synthesis route:

- $CO_2 + CH_4 \leftrightarrow 2\,CO + 2\,H_2$ (3)

Second, the direct route: the CO_2 is directly converted using electrocatalysis into platform chemicals such as methanol or ethylene. Third, the biological route: the conversion of locally produced small streams of biogas into methane or liquid products, for which efficient small-sale units are needed. Methanol is considered as an interesting platform chemical from which base chemicals can be produced and it also serves as a suitable transportation fuel (Olah's methanol economy). Efficient processes to activate ethane into useful base chemicals should also be considered (natural gas usually contains ethane that also has high value as chemical feedstock).

The second class of reactions of interest, starts with the production of hydrogen from water:

- $2\,H_2O \rightarrow 2\,H_2 + O_2$ (4)

This reaction also requires a large input of energy, while the hydrogen produced can be combined with reactions involving CO_2, to produce for example methanol or carbohydrates, or nitrogen to produce ammonia. The hydrogen-based reactions can be performed with existing processes and catalysts, although opportunities exist for process optimization. The last renewable reaction of interest is the production of ammonia following reaction (5):

- $N_2 + H_2O \leftrightarrow NH_3 + O_2$ (5)

To perform this reaction is extremely challenging, and in particular progress in the development of electrochemical methodology for this reaction is plagued by the underestimated role of N-containing contaminants in determining NH_3 yields. Most promising appear cycles on the basis of nitrides, combining thermal activation of N_2 to form nitrides, followed by conversion of the nitride with H_2O to ammonia. Whether such consecutive processes are economically feasible, remains to be determined.

The shift in feedstock will also lead to a shift in platform molecules in the chemical industry. For instance, expecting that synthesis gas will continue to grow in importance; requires novel (bio)catalytic processes to produce light olefins, the building blocks for plastics, directly from synthesis gas. The above innovations also require concerted developments in process technologies (engineering of (bio)catalysts, reactors, separation processes, etc.) to ensure high efficiency of the processes e.g. by controlling/shifting equilibria. In addition, development of more efficient separation technologies for mixtures of hydrocarbons based on principles other than the existing technologies may enable technologies at lower per pass conversions.

3.1.2 Feedstock diversification: Sustainable resources, electricity, light, others

Rather than a chemical industry based on fossil resources, a transition is required to renewable feedstock. Biomass is attractive for production of functionalized molecules, as will be addressed in paragraph 3.3.

Solar heat

To allow reactions (1), (3) or (4) (see previous paragraph), input of heat alone has been attempted by making use of so-called solar towers, in which solar light is concentrated and temperatures higher than 1000 °C can be reached. This is sufficient to perform reaction (4) with the help of a metal/metal-oxide cycle to generate hydrogen and oxygen in separate compartments of the tower. While several towers exist in, for example, the US and Spain, for the Netherlands solar towers are unsuitable to achieve conversion, since clouds are detrimental to the process, and clear skies are rare in the Netherlands.

Photocatalysis

Another technology which has been under development for decades, is to make use of light activated semiconductors in the conversion of water to hydrogen (reaction (3)). This technology is known as heterogeneous photocatalysis (liquid/solid reactors have been developed). For years the development of the technology has been dominated by the search for stable, visible light sensitive semiconductors, in combination with suitable, nanoparticulate “co-catalysts” to reduce the energy barrier of electron transfer reactions for hydrogen, and more importantly, oxygen formation. Thus far, it has proven unsuccessful to prepare stable, visible light sensitive semiconductors with high apparent quantum efficiency (AQE), i.e. the ration between the number of hydrogen molecules produced and the normalized number of photons to which the semiconductor-containing photoreactors are exposed. Typically this does not exceed 1%, while photocatalytic rates do not exceed $1\ \mu$ mole $g^{-1}\ h^{-1}$. A major recent achievement is the development of UV-sensitive semiconductor/co-catalyst systems, with close to unity in AQE. To upscale UV-based photocatalytic hydrogen production, efficient pilot reactors need to be developed, for example similar to systems used in ‘vertical farming’, making use of artificial, UV-LED light sources, fed by renewable electricity from wind and solar. The use of UV-LED minimizes energy losses, and allows operation 24/7, while direct solar illumination intrinsically implies the reactor and process are only operative for an approximate 6 hours per day in The Netherlands, strongly affected by seasonal fluctuations.

Photothermal catalysis

In recent years (combinations of) reactions (1) and (3), but also methane steam reforming and dry reforming, have been successfully performed by development of catalysts which are both photocatalytically, and thermally activated. Gas-solid reactors have been proposed, which allow simultaneous introduction of heat and visible light. Two variations of this technology have been proposed: i) A semiconductor (comparable to conventional catalyst supports such as TiO_2 or CeO_2) is light-activated, providing the necessary thermodynamically required energy input, and (similar to liquid-solid heterogeneous photocatalysis) nanoparticulate catalysts are thermally activated to overcome kinetic barriers of electron transfer reactions. Interestingly, the AQE appears to increase at elevated temperatures (a few 100s of degrees above room temperature). ii) plasmonic particles are deposited on conventional catalysts for hydrogen mediated reactions (such as the reversed water-gas shift reaction). Here, the plasmonic particles upon light absorption induce local, additional heating of catalyst particles, reducing the

energy input required for external heating of the reactor. For example solar through reactors have been proposed for upscaling, but this has not been practically performed, and the catalytic data are predominantly based on publications of a few research laboratories, and need to be verified.

Electrocatalysis at mild temperatures (hydrogen fuel cell-based)

Electrocatalysis can bring great opportunities for greening industrially relevant processes. Electrochemistry can drastically reduce the CO_2 footprint for a broad range of processes. Electrochemistry is of relevance for the production of hydrogen, CO_2 derived reduced materials, and in the further future ammonia from nitrogen and water (see reaction 5). Electrochemical engineering is one of the key elements which is needed to be able to fulfill the role within the energy and material transition. Typical electrochemical related challenges are to enhance:

- Current density
- Lifetime of materials
- Faradaic efficiency
- System design

High temperature electrocatalysis (solid oxide based)

Solid oxide electrolyzer technology is of relevance for producing hydrogen from steam, syngas from CO_2 and steam (so-called co-electrolysis), and CO from CO_2. The main advantage of the SOE technology is that a lower energy consumption is needed for the transformation due to the elevated temperatures. This technology can be further integrated (including by heat exchange) with industrial processes. The challenge is amongst others scaling up and improving durability and reliability.

Photoelectrochemistry

Another hybrid technology is the use of light-sensitive electrodes in electrochemical synthesis of platform molecules from CO_2, H_2O and N_2, known as photo-electrochemistry. The advantage of using photosensitive electrodes, is that part of the voltage that is required to supply the thermodynamic and kinetic input for the previously discussed electrochemical reactions, is provided by light. In other words, this is an integrated alternative for a separated PV system converting light to electricity, coupled to an electrolyzer converting electricity to chemicals. Research on the low TRLs is performed in various laboratories throughout Europe, including in The Netherlands. Here, besides completely inorganic chemistry and semiconductor based systems, also organic, bioinspired light absorbers and homogeneous catalysts, are developed. The challenge is to find robust molecules and electrodes, to extend the lifetime of such cells. Furthermore, very little studies exist attempting the scale-up of photoelectrochemistry.

Plasma catalysis

Plasma catalysis has recently gained traction, in particular as an alternative to ammonia synthesis (reaction (5)). The current research is mostly fundamental and little attention has been given to the technical and economic feasibility of plasma-catalytic ammonia synthesis. The technology appears most feasible for small-scale ammonia synthesis. Plasma catalysis potentially has a fast response to intermittent renewable electricity, although low pressure absorbent-enhanced Haber-Bosch processes are also expected to resilient to load variations. Low-temperature thermochemical ammonia synthesis is expected to be a more feasible alternative to intermittent decentralized ammonia synthesis, than plasma-catalytic ammonia synthesis due to its superior energy efficiency. Moreover, plasma technology can as well be used to reduce CO_2 to value added materials (eg CO). Process intensification and integration with other process steps can lead to a further overall improvement.

3.1.3 Efficiency in chemical production

The emerging fields of technology related to feedstock diversification, circular chemistry, as well as chemistry using biobased feedstock, will have to rely on a strong competency in catalysis, process technology and synthesis. Yet, beside as an enabler for these new directions, it is also these competencies that will be needed to on the short term reduce carbon footprint and improve efficiency in already exisiting chemical production routes and processes.

Catalysis

Development of new catalysts will be key in e.g. the C_1 chemistry as is proposed, but clearly also the routes using electricity and light will call for (new types of) catalysts. Beside this, already currently 85% of all chemicals made through existing processes are made catalytically. Improvement of catalyst activity and selectivity will lead to instant reduction in energy use and waste of raw materials.

While improved catalysts are needed to deal with current fossil feedstock that are generally becoming heavier and richer in contaminants, also the introduction of recycled feedstock and biobased feedstock requires new catalysts to treat these and enable integration into the existing value chains. While catalyst development is needed to improve efficiency of processes based on syngas, also routes to olefins involving dehydrogenation will see need for new and improved catalysts.

Furthermore, the scarcity of the catalytic materials used leads to a desire for more efficient recovery of the metals as well as an interest in using less noble and more abundant metals in catalysis. The Netherlands combines a concentration of catalyst producers and users, and world-class academic research groups in heterogeneous and homogeneous catalysis. Research on catalyst synthesis and focus on understanding the functioning of the catalyst using new and advanced characterizations and operando methods, will remain of key importance.

Reactor design

The upcoming transitions in the process industry also have important consequences for chemical reactor engineering as a discipline, and require novel research directions in this area. A more intermittent energy supply and more varying feedstock will enforce that reactors can deal with dynamic operation and complex flows. Process intensification will remain in important area, developing reactors that have integrated other functions, such as separation, next to the chemical reaction. Novel ways of supplying energy to reactors (electrocatalysis, photocatalysis, plasma, high-gravity) will find their way from the laboratory to industry. Structuring of reactors will increasingly be applied, since this can either boost the efficiency (e.g., higher mass transfer) or because the energy supply requires this (e.g., electrode plates).

Process Systems Engineering

Process Systems Engineering (PSE) takes a holistic view of chemical based manufacturing processes. Methodologies are systematically developed to support decision-making in a complex environment to optimally plan, design, operate and control chemical processes. For a truly sustainable technology the decisions should be based on economic, ecological and social implications. The boundaries of the system can be chosen different in space (a chemical plant, an industrial complex, a company, the industry, ..) and time (tomorrow, a quarter, plant life time ..). The continuing increase of availability of (process) data and computer power is the key enabler to the application of PSE to chemical processing. PSE contributions and developments in 5 areas are foreseen: 1) smart process modeling where the concept of artificial intelligence and digital twinning is fully used, 2) uncertainty assessment including advanced data analysis, 3) multi-criterion decision-making, 4) algorithmic solution methods that can be used to design and operate the future interconnected process systems 5) the overall integration, the implementation, sharing and valorization of the tools via the creation of human capital.

Heat remains a very important area of attention. It represents 80% of present industrial energy use. A thorough understanding and insight in this field is as essential as ever before. Within this framework heat integration in industrial processes using a classical pinch methodology is no longer enough. This can lead to the direct use of electrical power for high temperature processes and subsequent energy extraction through power generation combined with lower temperature heating medium.

Process Automation of the future processes will need to be adaptive to a variety of no longer fixed inputs. These are found in varying feedstock mixes, energy supply profiles as well as more specific and tailored demands from markets. The boundary between batch and continuous processes will blur and process automation and safeguarding will have to perform in any state the process is in. This will call for multi-level and dimensional data integration from physical equipment to anyone in need of interaction with the process with full data integrity and security. AI, VR, AR will play ever increasing roles in areas such as direct operations, training, safety, maintenance, quality and reliability

Separation

For the high volume production applications approximately 50% of the total production costs are caused by separation, so the applied technology is a very important aspect in a wide range of industries, including but not limited to the energy sector, the water sector, the chemical industry, and agro, food and feed. Separation technology is indispensable because there is no single process where a pure product is produced at 100% selectivity and 100% yield.

The main challenges for the discipline include: 1) Reducing as much as possible the dependence on fossil fuel as carrier of the energy converted into the thermodynamic separation work, in order to also reduce the emission of CO_2 and other greenhouse gases. This may be achieved by approaching the thermodynamic minimum energy demand as close as possible, but also by replacing the driving force by a more sustainable one. Examples include electric driving forces that can be powered with green electricity. 2) Becoming more flexible and able to handle streams with an increasingly complex nature, as required by the circular economy ambitions. These have a variety of origins such as in recycle- and bio-steams.

Another important area demands surgical separation of delicate molecules to preserve their properties and value. These are found in food processing with an increasing focus on nutritional value. Similar processing requirements are valid for pharmaceutical applications.

3.2 Making molecules circularly

3.2.1 Design for circularity

Within this important area of innovation, three domains can be recognized: systemic innovations in a value network, design for circularity and also design from circularity.

A transition is required from the current linear value chains into value networks, where industrial and post-consumer waste becomes a feedstock for the chemical industry. This transition starts with obtaining insight in the current system, followed by the development of a multi-criteria (techno-economic, social, ecologic, environmental) scenario-based decision-tool that allows for evaluation of the impact of policy, incentives, technology, circular feedstock & products, supply-demand, etc. on circularity. Finally, the outcomes of such a tool can be used for roadmapping of concrete steps forward.

Design for circularity is focused on the development of better materials and products, that simplify recycling (both mechanical and chemical), whilst maintaining their intended functionality. For this purpose, current and future sorting and recycling technologies should be taken into account when designing new plastic products. For instance, packaging currently consist of multi-layers (e.g. bread-bag consists of 50 layers of PE) and/or multi-materials (e.g. meat-trays consists of different components: tray, sealing, lit; composed of different materials). Such products should be transformed into mono-materials and/or mono-layers leading to easier separation at recyclers, which in turn results in less losses. From a chemical recycling perspective, polycondensates (such as PET, PLA) are more suitable materials compared to the polyolefins currently used at large scale; hence the enhanced use of polycondensates for single-use plastics and packaging should be promoted. At the same time, development of better (chemical) sensors and application of AI and machine learning will also lead to improved sorting and less waste of the more complex products. Finally, special attention will be required for those products that contain additives (e.g. WEEE plastics).

Design from circularity is focused on the development of techniques for use of sorted waste streams for the production of existing and novel plastic products. Currently, more than 50% of recycled product can only be used for low-value applications (PE-bench instead of packaging), due to coloring, haziness or contaminants (e.g. legacy-molecules). With design from circularity novel high-value applications will be developed, that in turn can easily be recycled. As such design from circularity is complementary to design for circularity.

3.2.2 Circular polymers

The current situation on polymer recycling relies on two main approaches: mechanical recycling (aim at winning the material back from waste streams) and chemical recycling (mainly aiming at winning valuable chemicals, including monomers whenever possible, by chemical degrading the polymeric chains). From a scientific point of view, three main topics still require particular attention in terms of developing new concepts on a fundamental level:

I. recycling of crosslinked structures (rubbers and thermosets);
II. upgrading the current recycling approaches for thermoplastics suffering relevant side-reactions during processing (for example degradation);
III. combining different waste streams into polymer blends possibly to be optimized via reactive extrusions strategies.

This stems on one side form the current relevant shortcomings in the corresponding technological approaches while, on the other hand, it requires significant advances (for example sensor technologies) in the physical separation and collection of post-consumers waste streams.

After collection and physical separation, meticulous characterization is needed in order to identify the impurities remaining in the material. Low molecular weight compounds should be identified as to propose suitable separation techniques (both before and after collection and physical separation), which should then be attractive at industrial scale. This might disclose on the longer term application of relevant streams for added values applications where the absence of any unwanted impurities is paramount. On the other hand, in case the pollutant is another polymer, identification of the kind of material (simple polymer blend as opposed to co-polymers) is crucial in devising further strategies. A simple blend can in principle still be separated in individual components although the classical approach (at academic level) of selective solvent extraction is clearly not suitable at industrial level and new more efficient and less energy demanding strategies should be defined and researched. Along the same line, one could think of proposing similar separation strategies for composite materials with no chemical bond between the matrix and the filler. On the other hand, a copolymer cannot per definition being simply separated in the individual blocks. Straightforward application of these materials as compatibilizers for polymer blends might be then considered a valuable option that dovetails strategy III (*vide supra*). Identification of other application routes for these copolymer should be further investigated.

On a more general level, integration of the “supply chain” for waste materials both from postconsumer as well as industrial streams seems to be a *conditio sine qua non* in order to define, among others, decision models for the allocation of given waste streams for mechanical and/or chemical recycling. Last but not least, when dealing with post-consumer waste, it is worth noticing how the relative production volumes still point to few class of polymers (polyethylene, polypropylene, poly(vinyl chloride), polystyrene etc.) as the major contributors, in volume, to the waste. In this context, it would be strongly desirable that the research points and strategies outlined above would also, if not predominantly, be referred to this class of bulk polymers.

3.2.3 Circular critical elements

Conservation of our elementary building blocks is needed to ensure their application in sustainable technologies, prevent chemical pollution and preserve biodiversity. This can only be carried out by recovery and recycling them after their use. The development of chemistry that enables the circular use of our elements, molecules and materials is therefore key, next to preventing chemicals from entering the environment, and thus avoiding them to cause pollution. Safe and circular by design of molecules and materials for a sustainable future is thus of utmost importance. Inducing such change from the current linear ‘take-make-dispose’ model to a more circular one requires a holistic approach to design a new system of using and reusing our precious elements.

The Critical Raw Materials List (CRM) of the European Commission contains 30 materials (Antimony, Baryte, Beryllium, Bismuth, Borate, Cobalt, Coking Coal, Fluorspar, Gallium, Germanium, Hafnium, Heavy Rare Earth Elements, Light Rare Earth Elements, Indium, Magnesium, Natural Graphite, Natural Rubber, Niobium, Platinum Group Metals, Phosphate rock, Phosphorus, Scandium, Silicon metal, Tantalum, Tungsten, Vanadium, Bauxite, Lithium, Titanium, Strontium), of which the last four are added in 2020 to the list for the first time. In the coming years, the availability of those critical raw materials is under stress and the mining will eventually reach peak production, like it was observed for oil. Recovery and recycling will become more important and chemical recycling techniques will be required.

Many scarce metals and materials are critical for the Dutch and EU industry, in particular for the high-tech and clean energy applications. Examples of these critical materials include: rare earth elements in particular neodymium (Nd) and dysprosium (Dy) in permanent magnets for electric motors/generators in wind turbines and electric vehicles; cobalt and lithium for Li-ion rechargeable batteries for electronic products/equipment and electric vehicles.

Industrial recycling value chain involves three interconnected steps: collection, physical separation, and chemical/metallurgical refining. At present, The Netherlands is among the front runners of the collection system and infrastructure for most of the waste and end-of-life (EOL) products, and has quite mature physical separation industry with advanced technologies such as ARN for collection and physical (or mechanical) recycling of EOL vehicles or ELVs, Renewi and SIMS recycling for physical recycling of electronic waste. However, there is a clear knowledge and technology gap for efficient separation and extraction of these critical materials. The main challenge lies in their dilute use as “minor constituents” in the bulk materials (e.g. minor alloying elements, coatings), or relatively small or tiny components in a large equipment or product.

Biochemical elements like carbon, nitrogen and phosphorus face different challenges. The disposal of these elements have pushed four of the sustainability targets (Steffen, Rockstrom et al. *Science* **2015**, *347*, 736) into unprecedented territory, namely: extinction rate (one of two indicators for biosphere integrity), atmospheric carbon dioxide (an indicator for climate change), and the biogeochemical flow of nitrogen and phosphorus, of which the latter three can be solely ascribed to the chemistry of three elements: (C, N, P). Urgent action therefore needs to be taken to return to safe operating space in these processes.

Therefore, next to advancing resource management, sustainable chemistry is also urgently required to tackle environmental waste issues. For carbon, this mainly concerns the greenhouse gases carbon dioxide and methane that are expelled to the atmosphere. The nitrogen waste issue is caused by nitrogen oxides (N_2O, NO_x) and predominately ammonia (NH_3) that are discharged into the aquatic environment and/or atmosphere. For phosphorus, it concerns phosphate, which is next to ammonia essential for plant growth, yet this building block of life also ends up in aquatic systems causing eutrophication. Ironically, C, N, and P are key players in the suite of major biogenic elements, often termed 'CHONPS', needed in large quantities to make living organisms, but also contribute heavily to three of the most stringent environmental concerns.

3.3 Making molecules from biomass

3.3.1 Biorefining

Bio-based feedstock (e.g. biomass) is a renewable (sustainable) heterogeneous resource consisting of functional molecules (polysaccharides, lignin, proteins, lipids) formed by nature out of CO2, water, nutrients and sunlight. Bio-based feedstock are used since the dawn of mankind for e.g. food, feed, heat and construction materials. More recently it was realized that bio-based feedstock could also be a sustainable source for chemicals, fuels and materials like polymers. However, care has to be taken that its use for these purposes does not compete with its use for food and feed (i.e. the food vs fuel discussion).

To make efficient use of the molecules present in bio-based feedstock, a biorefinery approach to efficiently separate the different components and, when needed, convert them further to the desired products, is needed. When doing so three prerequisites have to be satisfied:

1) do not endanger food/feed production;
2) use the feedstock to its highest value;
3) make molecules/products which can be recycled (i.e. connect to a circular economy) or that replace fossil-based products that cannot be recycled (e.g. paints, coatings, lubricants, rubber, etc.).

Although examples exist of high TRL biorefinery approaches and of products that even made it to commercialization (e.g. polylactic acid), the large scale use of biorefinery approaches which can outcompete the large scale use of fossil resources in an oil refinery is limited. This is mainly related to the low yields, high energy inputs and too specific approaches for each bio-based feedstock which all relate to the complex nature of bio-based feedstock. Here clear improvements need to be made. This does not only require new scientific and technological breakthroughs, but it also requires new value chains in which 'unconventional partners' like bio-based feedstock producers, food industry and chemical industry collaborate.

To achieve the use of bio-based feedstock on a large and economically viable scale different steps need to be made:

1) Application of novel (bio-)catalytic processes that reduce the high energy inputs and increase the yields of biorefinery operations, whilst working with a variety of (less pure) bio-based feedstock. Since (bio)catalysis is a core element it will be discussed separately.
2) Development of new biorefinery and separation technologies to produce products based on their required functionality rather than on their purity. This is expected to result in lower energy input and less processing steps.
3) Development of new value chains that use bio-based feedstock without endangering food/feed production.

3.3.2 (Thermo)-Chemical biomass conversion

To valorize dry biomass via (thermo-)catalytic conversions three main routes are envisioned, all of which contain catalytic steps i.e., the syngas route, the pyrolysis route, and the moderate temperature route. The first two routes break down the biomass either to syngas (CO and H_2) or bio-oil (complex mixture of molecules). For the further conversion of these streams similar processes as developed for fossil feedstock can be used. However, these processes have a special edge related to catalyst stability. The third route maintains as much as possible the functionalities (atom efficiency) present in the biomass. The latter route needs significant more research input compared to especially the first route, also from catalysis and downstream processing, to convert the complex biomass mixture to desired molecules. Yet, since the biomass is highly functionalized, this route is very promising for making (bulk and functional) chemicals.

3.3.3 Biomass conversion using industrial biotechnology

Industrial (White) Biotechnology is an important tool to process dry and wet biomass in a wide array of chemicals and fuels. A clear distinction can be made between fractionation of biomass, enzyme development for hydrolysis of recalcitrant biomass (e.g. lignocellulosic materials), and fermentation and enzymatic processes for production of chemicals and fuels. The Netherlands has a forefront position in industrial biotechnology both on an academic level as well as in the industrial landscape (among others DSM, Dupont Industrial Biosciences, Dutch DNA, Corbion, Paques, Dyadic Netherlands, Photanol). In addition, there is excellent expertise in the production of bulk/platform chemicals from organic waste and side streams (Paques, Orgaworld, Royal Haskoning DHV, Veolia and others).

To fully explore the potential of industrial biotechnology for the conversion of biomass it is important to:

1) Discover novel biocatalysts, including isolation/development of novel microorganisms/microbiomes for industrial applications (considering needs in terms of substrate and desired product, as well as desired industrial process conditions). Improve microbes/microbiomes using synthetic biology approaches (application of state-of-the-art genome editing tools and systems biology approaches).
2) Screen extremophiles, as whole-cell biocatalysts or for their enzymes (including high and low T, high salinity, high and low pH, etc.).
3) Study novel bio-catalytic processes for the production of chemicals that are difficult to produce with chemistry, such as some polymers (intra- and extracellular), biosurfactants, and feed and food additives.
4) Develop integrated fermentation platforms (mixotrophic fermentations, one-carbon based fermentations, bioelectrochemical fermentation) for complete use of biomass potential, together with downstream process technology.

3.4 Making functional molecules

3.4.1 High performance materials

High performance polymeric materials are generally characterized by significant levels of purity (a “must” for a correct product design) as well as the presence of the relevant functional groups needed for the specified performance. This entails the controlled and precise synthesis of novel polymeric structures and/or modification of existing ones. Against this backdrop and making allowances for a general sustainability (and circularity) driven context, it is possible to revision a main theme around the use of biobased monomers and/or *functional* molecules derived from chemical recycling (e.g. pyrolysis) approaches. This requires a shift in the attention from a technological push (from new monomers to applications) to market pull. The latter should start defining the required performance, translate that into quantifiable engineering characteristics and properties for the material up to the envisioned chemical structure and the monomers selection form the two classes specified above. A more short term approach would rely on the precis modification of recycled materials possibly based on “commodity” polymers. This resembles many efforts spent in the 80’s and 90’ both at academic and industrial level to upgrade bulk polymeric materials (for example polyolefins) to high performance ones via chemical modification. However, the use of recycled polymers as raw materials poses a series of challenges in terms of quality of the recycled polymers (partially addressed in the section above on circular polymers) as well as in terms of new strategies for the required chemical modification.

3.4.2 Specialty, pharma and fine chemicals

In the synthesis and manufacturing of (often complex) small molecules, three domains of major challenges exist . Interconnected challenges exist in the areas of :

1) Sustainability, hazard (process and products), health and environmental issues.
2) Predictable design and improvement of products (molecular structure -function) and processes.
3) Changing the paradigm of global outsourcing in manufacturing and observed associated societal risks

1. Many processes for making complex functional small molecules still use large quantities of reagents with tedious protective group strategies to achieve selective functionalization. As a result, the synthetic procedures often generate one hundred times more waste than desired product. To improve the existing synthetic processes and to accelerate the discovery of new transformations, significant breakthroughs in synthesis and catalysis are required. Although important advances in the field of catalysis have been achieved in academia in recent years, the major implementation challenges still remain, . To address these challenges, synthetic research should be directed towards a fundamental understanding of chemical reactivity and processes, the development of conceptually new synthetic methods, and the introduction of novel, smart, robust, promiscuous and, above all sustainable catalysts based on rational design. Going forward, a (re-)connection of the synthetic armory to a largely renewable/circular building blocks basis is also a ‘must do’.
2. In various use domains of specialty chemicals continuous effort is required to better understand and predict the function – molecular structure relations. This will allow more rational product design. However, also consequences such as the environmental impact – product structure & process relations, need much improved scientific basis and predictability. Especially significant AI/ML (Artificial Intelligence/Machine Learning) methodology will enable step drastic changes in synthetic route- design and manufacturing process optimization. For formulated, specialty products not only the purity but also the form like the particle size or shape is important.
3. In a societal painful manner (e.g. COVID-19 related examples)the lesson is being learned that access to complex chemicals derived from long – global - value chains, purely driven by direct costs sets the society at great risk. Decentralized, regional/local manufacturing infrastructure at acceptable costs has to be re-established. Further developments in PI , both in the reactor sections as well as in the downstream separation units, will greatly facility re-establishment of regional/local manufacturing at acceptable costs and with maximal societal security of supply benefits. The field of modular, efficient separation and purification is currently underdeveloped compared to modular reactors. Modular, small reactors and (separation) unit operations , including access to high T/p-reaction domains, and including full automated control are required. Realizing all of this requires inclusion of ‘on demand’ (3-D printing) technologies for such equipment.