SUSCHEM
European Technology Platform
for Sustainable Chemistry

Strategic Innovation and Research Agenda

Innovation Priorities for EU and Global Challenges

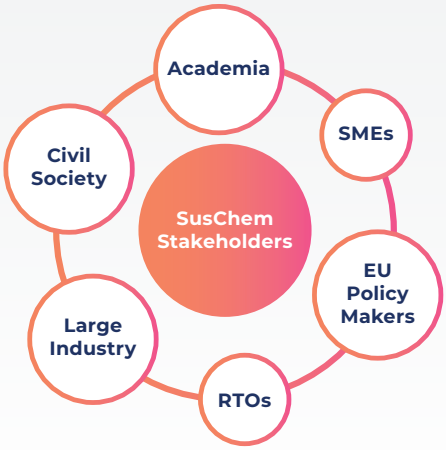
www.suschem.org

SusChem Mission

SusChem's vision is for a competitive and innovative Europe where sustainable chemistry and biotechnology together provide solutions for future generations. SusChem's mission is to initiate and inspire European chemical and biochemical innovation to respond effectively to global challenges by providing sustainable solutions.

The common objectives between the SusChem ETP and SusChem NTPs network include:

- Bringing together industry, academia, civil society and national governments to address European and global challenges and improve industrial competitiveness;
- Contributing to develop an EU-wide common strategy to support the position of the chemical sector with the European Commission and other European Institutions ("bottom-up" approach);
- Aligning priorities of the ETP and of the NTPs to gain broader support (complementary "top-down" activity);
- Facilitating transnational collaboration within research and innovation projects and the international transmission of skills;
- Facilitating networking, cluster creation, project teams, etc. to enhance participation in EU funding programmes, especially for SMEs.



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Special thanks go to all SusChem Board members and all representatives of the SusChem National Technology Platforms (NTPs) network for remaining consistently engaged in ensuring the strategic direction and vision of the new SIRA as well as for connecting the SusChem project team with their network of experts.

The production of the new SusChem SIRA would not have been possible without the direct contribution of over 100 experts across universities, Research and Technology organisations (RTOs) as well as SMEs and the large industry. These experts contributed through the initial consultation rounds, a workshop to define the final priorities and by formulating sections of the new SusChem SIRA. Moreover, we would like to thank PNO Consultants for their contribution in structuring and further developing the content of the new SIRA document.

So many experts and organisations have contributed at different levels that we cannot thank all of them specifically. Yet the quality of their input is reflected in this ambitious SIRA.

We sincerely hope that we will continue working with all stakeholders to take this agenda forward.

Version November 2019

SUSCHEM

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Foreword

Mitigating climate change, protecting our limited natural resources, combatting environmental pollution, making best use of the unprecedented digital opportunities; challenges like these are shaping the global agenda at a breathtaking pace. Answers to such challenges can greatly stem from innovative solutions based on sustainable chemistry: the core of the European Technology Platform for Sustainable Chemistry (SusChem ETP).

Founded 15 years ago, SusChem has become an ambitious and impactful technology platform at European level. Key to success is our spirit of collaboration and openness to a broad range of stakeholders – comprising the large industry, small and medium-sized companies and startups as well as Research and Technology Organizations (RTOs) and the academic world. Furthermore, the commitment and involvement of civil society has been an indispensable cornerstone to realize our vision of advancing sustainable chemistry via research and innovation. In order to get there, we build on an interdisciplinary approach, including process engineering, industrial biotechnology, materials science, digital technologies and other domains.

The framework conditions are both demanding and supportive. European policy makers are striving for positioning the European Union at the forefront of sustainable development. I would like to mention the "European Green Deal", as envisaged by the new President of the European Commission, Ursula von der Leyen, as well as her vision of a "Europe fit for the digital age". Such a future-oriented agenda sets ambitious targets for Europe by 2030, including a new Circular Economy Action Plan, a zero-pollution strategy and the first European climate law as well as a new industrial strategy. Additionally, there is an increased consideration of digital technologies for enabling solutions to industrial and societal challenges.

We embrace the continuous and strong support by the EU Commission on research and innovation. And we are very much looking forward to the next research and innovation programme "Horizon Europe" which will start in 2021 for another seven-year period. It will surely support the necessary innovation to address major challenges both on a European and global scale, through accelerating cutting-edge research, from fundamental research to pilot and demonstration projects that will eventually also increase the competitiveness of the European chemical sector.

SusChem has now reached its next milestone: our new Strategic Innovation and Research Agenda (SIRA). Being the result of a co-creation process together with our stakeholders, it outlines our strategic priorities towards 2030, with links to Horizon Europe and beyond. The new SIRA reaffirms sustainable chemistry in an even more ambitious way, towards achieving cross-sectorial breakthroughs through novel and sustainable processes and products. It focuses on technology priorities across advanced materials, advanced processes as well as the implementation and co-development of enabling digital technologies.

To realize our overarching goal, which is the transformation of research into innovation, we support development at all technology readiness levels – from fundamental research to pilot and demonstration projects. The SusChem community also underlines under the new SIRA the importance of advancing in parallel on sustainability assessment, safe-by-design for chemicals and materials and building further on the education and skills capacity in Europe.

The momentum and success of the new SIRA will be highly connected with the commitment of SusChem stakeholders. I would also like to thank the more than 100 SusChem experts who contributed to the formulation of the new SIRA. However, to effectively address grand challenges, such as the transition to a more circular economy, we also need the involvement and collaboration of stakeholders throughout the value chain and across various sectors to the greatest possible extent, complemented by societal awareness and acceptance. SusChem will also continue its fruitful collaboration and trustful relationship with the European Commission, driven by the joint target of securing the leadership of our continent in terms of technology and innovation.

I am convinced that the new SusChem SIRA will further enable and stimulate the chemical sector to find the right answers to the pressing challenges our world is facing as well as satisfy the ambitious political objectives for Europe. And I very much hope that it will result in boosting the competitiveness of our sector at national and EU levels.

Dr Markus Steilemann,
Chairman of SusChem ETP,
CEO of Covestro AG

1 INTRODUCTION

SUSCHEM

SusChem Priorities: Technologies for a Better Future of Europe

Moving towards 2030, SusChem recognises three overarching and interconnected challenge areas: Circular economy and resource efficiency, low carbon economy towards mitigating climate change, as well as protecting environmental and human health.

This will require aligning all actors of the innovation ecosystem on priorities, across value chains, and spanning from the most fundamental to the most advanced technological readiness levels.

CIRCULAR ECONOMY AND RESOURCE EFFICIENCY

Transforming Europe into a more circular economy

- Materials design for durability and/or recyclability
- Safe-by-design for chemicals & materials (accounting for circularity)
- Advanced processes for alternative carbon feedstock valorisation (waste, biomass, CO/CO_2)
- Resource efficiency optimisation of processes
- Advanced materials and processes for sustainable water management
- Advanced materials and processes for the recovery and reuse of critical raw materials and/or their sustainable replacement
- Industrial symbiosis
- Alternative business models
- Digital technologies to increase value chain collaboration, informing the consumer and B2B on reuse and recyclability

LOW CARBON ECONOMY

Mitigating climate change, with Europe becoming carbon neutral

- Advanced materials for sustainable production of renewable electricity
- Advanced materials and technologies for renewable energy storage
- Advanced materials for energy efficiency in transport and buildings
- Electrification of chemical processes and use of renewable energy sources
- Increased energy efficiency of process technologies, enabled by digital technologies
- Energy efficient water treatment
- Industrial symbiosis via better valorisation of energy streams
- Alternative business models

ENVIRONMENTAL AND HUMAN HEALTH

Europe leading on environmental and human health protection

- Safe-by-design for materials and chemicals (functionality approach, methodologies, data)
- Improve safety of operations through process design, control and optimisation
- Zero-liquid discharge processes
- Zero-waste discharge processes
- Technologies for reducing GHGs emissions
- Technologies for reducing industrial emissions
- Sustainable sourcing of raw materials
- Increasing transparency of products within value chains through digital technologies
- Alternative food technologies
- Novel therapeutics and personalised medicine
- Sustainable agriculture, forestry and soil health related technologies
- Biocompatible materials for health applications

SUSTAINABILITY ASSESSMENT INNOVATION

EDUCATION AND SKILLS CAPACITY

ENABLING DIGITAL TECHNOLOGIES

Sustainable Chemistry: Innovation in a Rapidly Changing Environment

Chemistry has supported the development of the high standards of modern societies. Chemical products, building blocks and materials are indispensable to almost all value chains and industries, from automotive, aeronautics, electronics, energy, construction, textiles, pulp and paper, to healthcare, agriculture and food. Sustainable chemistry being such a key enabler for the entire economy, has a major role to play to drive the changes and develop solutions to address pressing global challenges, such as climate change, the need for a more circular economy, the smarter use of resources, and environmental and health protection.

Sustainable chemistry is at the heart of the SusChem European Technology platform (ETP). "Sustainable chemistry encompasses the design, manufacture and use of efficient, effective, safe and more environmentally benign chemical products and processes".[1] It also enables the development of technologies that boost the competitiveness of the chemical industry, whilst stimulating innovation across other sectors to design and discover new and sustainable products. It is enabled by interdisciplinary scientific and technological developments, beyond the strict traditional boundaries of chemistry, such as process engineering, industrial biotechnology, materials science, digital technologies, and many other domains.

Europe is the world's second largest chemical producing region, with an annual turnover of €542 billion (2017).[2] It provides 1.2 million direct jobs and it is the third largest investor in EU manufacturing (€21.6 billion, 2017).The European chemical industry is very diversified and spans from commodity chemicals through to specialty and fine chemicals including basic and versatile building blocks from fine and specialty chemicals, such as active pharmaceutical ingredients. The share of industrial biotech-related employment in total chemicals and pharmaceuticals as of 2013 amounted to about 5 % and is anticipated to increase to between 10 % and 15 % by 2030.[3]

ADDRESSING INNOVATION THROUGH KEY ENABLING TECHNOLOGIES (KETS)

In the Horizon 2020 research and innovation programme, the EU invested in six Key Enabling Technologies (KETs) for a sustainable and competitive European industry:

1. Nanotechnology
2. Micro- and nano-electronics
3. Photonics
4. Advanced materials
5. Advanced manufacturing technologies
6. Biotechnology

A high-level group on industrial technologies advised that the European Commission supports the six KETs as follows:

- Advanced manufacturing technologies
- Materials and nanotechnology
- Photonics and micro-/nano-electronics
- Broadening the KET 'biotechnology' to 'Life Sciences'
- Artificial intelligence
- Digital security and connectivity

The European chemical sector has a strong capacity to innovate, responding to challenges and new market and societal demands. To effectively deliver on the full potential of technological innovation, a coherent policy framework is required for implementation and market uptake. A key element of complexity for innovation, applicable to the chemical sector, is linked with the variety of types of processes, a broad range of products, and energy intensity. Consequently, increasing circularity and establishing the low carbon energy transition requires a broad portfolio of key enabling technologies (KETs).[4] SusChem embraces KETs as the technology building blocks for advancing Europe and addressing global challenges. The integration between materials, processes and digital technologies will accelerate the energy transition, the development of a climate neutral circular economy, and the creation of new markets, growth, and jobs.

In the coming decades, life in Europe will be impacted by a set of global megatrends, defined as "a major shift in environmental, social or economic conditions that that will play out over the coming decades"[5] and will substantially change the way people live. Demographic changes, economic growth, environmental risks, technological development, and geopolitical megatrends will have the biggest impact on the world. Innovation from the chemical sector, including its full innovation ecosystem, will be essential to respond to these challenges. Furthermore, transparency and trust will become progressively more and more important with consumers demanding an enhanced understanding of how products are made as well as their full environmental footprint. Trust will be based on the assessment of the products over their full life cycle, through transparent and shared methodologies. Compliance with the framework of sustainable development, and notably circular economy, will be a must.

IMPACT OF SUSTAINABLE CHEMISTRY AND INDUSTRIAL BIOTECHNOLOGY ON GLOBAL CHALLENGES - UN SDGS

The most serious sustainability deficit and our greatest challenge for Europe is said to be its ecological debt; natural resources are being overused and depleted, thereby threatening our ability to meet the needs of future generations within the limits of our planet. Worldwide, the strains on key resources, from fresh water to fertile land, put human existence and environmental health at risk. Biodiversity and ecosystems are increasingly threatened and global greenhouse gas (GHG) emissions continue to rise at an alarming rate because of energy use and overconsumption of resources. The United Nations (UN) Sustainable Development Goals (SDGs) are a universal set of 17 goals with 169 corresponding targets, agreed upon by UN member countries to solve some of humanity's biggest challenges by 2030. They show the way to make the transition to a "more climate-friendly, green, fair and inclusive future". For several of these UN SDGs, sustainable chemistry and industrial technology will have direct and indirect contributions:

Practicing **Sustainable Chemistry** is about efficiency and reducing the environmental impact of processes and products, optimising the use of finite resources and minimising waste while also valorising waste and by-products. The direct impact at chemicals production level and indirect impact in the use and end-of-life of products will also contribute to other sectors. Beyond 'safe-by-design' for chemicals and materials to prevent harm for human and environmental health, the application of Sustainable Chemistry technologies at large-scale is a prerequisite for a **globally competitive**, **low carbon**, **resource-efficient**, and **circular economy**, whilst **protecting environmental and human health**.

The EU Strategic Directions Require Sustainable Chemistry

In the context of global challenges, the strategic directions set by European policy-makers position Europe at the forefront of sustainability. Europe's ambition is to become the leader in the transition to an economy that keeps growing within environmental and societal constraints. The communication of the President of the European Commission, Ursula von der Leyen,'A Union that strives for more – My agenda for Europe',[6] highlights six headline ambitions, amongst which 'A European Green Deal' confirms the willingness of the new European Commission to reinforce earlier ambitions such as the commitment of Europe to the Paris Agreement on Climate Change. Moreover, 'A Europe fit for the digital age' highlights the consideration of digital technologies to enable solutions to grand industrial and societal challenges.

Addressing the European objectives, in line with the ambitious timescales considered, will require breakthrough technologies and disruptive models at a scale and at a pace never encountered before, that will transform every value chain. The chemical sector will have to support this overall transformation of society and industry. This will only happen by taking advantage of all possible technological options, with a profound impact on chemical production itself: Better usage of mineral and organic resources, increased use of alternative feedstock, electrification of chemical processes, new catalytic processes, biotech-driven processes, new and innovative eco-designed materials and use of waste energy flows within the chemical industry and with other industrial sectors. Many current chemical processes and chemical production units will require retrofitting to become more sustainable and adapt to the digital era. At the same time, downstream industries will continue to rely on the chemical industry to deliver products, advanced materials and technologies that they need to fulfil their own objectives of GHG emission reductions and circularity. Overall, this requires significant investments in research and innovation across the Technology Readiness Levels (TRLs).

'A UNION THAT STRIVES FOR MORE': AN AMBITIOUS EUROPEAN AGENDA

Many of the key foreseen initiatives under **'A European Green Deal'** are relevant to Sustainable Chemistry and industrial biotechnology, through advanced materials and advanced processes, including:

- The new Circular Economy Action Plan, which will extend to new sectors such as textiles, food and Information and communications technology (ICT)
- The forthcoming new industrial strategy
- The European Climate Law, which will enshrine the 2050 targets into law
- The Farm-to-Fork strategy on sustainable food
- The Zero-Pollution Strategy

'A Europe fit for the digital age' indicates the strong contribution of enabling digital technologies. Specific targets include:

- Data and AI as ingredients for innovation to find solutions to societal challenges, from health to farming, from security to manufacturing
- Jointly defining standards for this new generation of digital technologies that will become the global norm
- Empowering people through education and skills

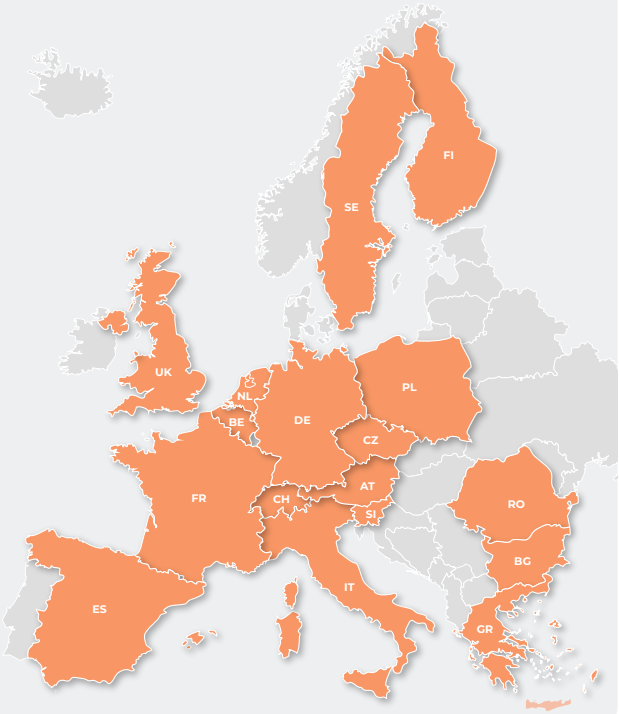
Building the new SusChem SIRA and the way Forward

This new SusChem SIRA is the result of a co-creation process that involved more than 100 experts, members of existing working SusChem groups and new participants, from large industry, academia (universities and Research & Technology Organisations (RTOs)) as well as SMEs, with national-level connections via the SusChem National Technology Platforms (NTPs). The process involved consultation rounds and a face-to-face workshop to define the final priorities, followed by the further engagement of the experts to formulate the new SIRA itself. The SusChem Board, with representatives from the full innovation ecosystem, remained consistently engaged in ensuring the strategic direction and vision of the SIRA.

The aim of this final document is to start a vibrant and constructive discussion with and between the SusChem stakeholders, EU policy makers and civil society. The new SusChem SIRA summarises the technology priorities that underline the contributions of chemistry to the journey towards sustainability. The development of these technologies entails the involvement and contribution of all concerned stakeholders. The Industry will continue to play an important role in the upscaling and deployment of novel technologies. The SusChem SIRA will be the basis for discussion with the public sector at all levels (EU, Member States, regions) to support this endeavour.

CONNECTING NATIONAL AND EU PRIORITIES IN THE NEW SUSCHEM SIRA: SUSCHEM NTPS

The SusChem network includes 17 National Technology Platforms (NTPs), capitalising on the synergies of its members to achieve its goals at European and National levels. EU Member States, each have different research and innovation capacities and face different challenges: SusChem NTPs help to define and communicate SusChem priorities, accounting for national and regional needs. SusChem NTPs have been key to the involvement of national stakeholders including small and medium-sized enterprises (SMEs), large companies and academic groups, towards defining specific technology priorities for 2030. Highlighted overarching priorities for the NTPs network encompassed: networking actions (including SMEs and start-ups), industrial symbiosis as well as building on skills and education for innovation uptake by both experts and civil society.



SUSCHEM STAKEHOLDERS: A CALL FOR ACTION

The mindset of SusChem stakeholders is positive and calls for action. Europe can harness the potential of further scientific and technological advances which stand at the core of society's search for solutions. Contributions are needed from all parts of society, but technology is a key driver. There is no easy way, no single company, no single industrial sector, that can do it alone. The whole community of SusChem experts is committed to take sustainable chemistry to the next level together with value chain partners. For SusChem and sustainable chemistry, the opportunity rests with the strong European R&I ecosystem including academia, a rich network of RTOs, small and large private companies including leading global chemical companies.

Innovation and EU Investment Tools – the SusChem Perspective

Ambitious political objectives have implications that affect different policy areas (e.g. environment, energy, climate change etc.). Innovation initiatives are triggered by different European and national programmes that help face the high risk inherent to such radical transformations, at different TRLs. It is necessary to ensure complementarity between and combination of different funding schemes at EU as well as regional and national levels.

At European level, **Horizon Europe (HEU) (2021-2027)** is a major programme to support innovation in Sustainable Chemistry and key enabling technologies. The Horizon Europe three Pillar structure is designed as follows:

Pillar I of HEU 'Excellent Science' and the European Research Council (ERC) are designed to strengthen cutting edge research through investing in highly skilled researchers in a wide range of disciplines relevant to SusChem e.g. Chemistry, Chemical Engineering, material Science and Biotechnology. Pillar I will also contribute to foster collaborations across different disciplines, promoting interdisciplinary research.

Pillar II of HEU 'Global Challenges and European Industrial Competitiveness' will foster EU industrial competitiveness and deliver on the EU's strategic priorities and tackle global challenges that affect the quality of our daily lives. Through its thematic approach, it will aim to:

- Accelerate from fundamental research in SusChem KETs to pilot and demonstration;
- Foster the Research and innovation synergies of universities, Research & Technology Organisations (RTOs) with large Industry and SMEs;
- Link the different industries in their developments, especially when targeting eco-designed products, circular economy, bioeconomy, and digitalised value chains. This should be driven through collaborations with different Public-Private-Partnerships (PPPs) and ETPs. It is important to build on the successes of existing initiatives such as the 'Bio-Based industries Joint Undertaking' (BBI JU) and the 'Sustainable Process Industry through Resource and Energy efficiency contractual Public-Private-Partnership' (SPIRE cPPP) and ensure their continuation.

Pillar III of HEU 'Innovative Europe' and the European Innovation Council (EIC) is designed to accelerate innovation, testing new ideas and technologies as well as business models to help bring innovations to market. SusChem supports the emergence of major and global new market players who develop breakthrough innovations, whilst it will continue to foster innovation collaborations between early stage innovators and industrial players.

HEU - European Research and innovation missions will be established for the first time under HEU with the aim of boosting the impact of EU-funded research and innovation by mobilising investment and EU-wide efforts around measurable and time-bound goals around issues that affect citizens' daily lives. The SusChem priorities in advanced materials, advanced processes and digital technologies, including Horizontal Topics (e.g. education/skills development), will be key enablers to successfully conclude the mission-oriented targets.

Beyond Horizon Europe (HEU), other funding instruments drive innovation in SusChem-related technology priorities

New LIFE programme (2021-2027) is dedicated to environmental and climate objectives (Nature and Biodiversity, Circular Economy and Quality of Life, Climate Change Mitigation and Adaptation, and Clean Energy Transition). Projects closely linked to SusChem, such as developing technologies for implementing waste and water management, safe-by-design or developing technologies focusing on energy efficiency, can benefit from LIFE.

Digital Europe programme (2021-2027) is focused on building the strategic digital capacities of the EU and on facilitating the wide deployment of digital technologies, to be used by Europe's citizens and businesses. The programme will boost investments in relevant SusChem areas including artificial intelligence, cybersecurity, advanced digital skills, and ensuring a wide use of digital technologies across the economy and society.

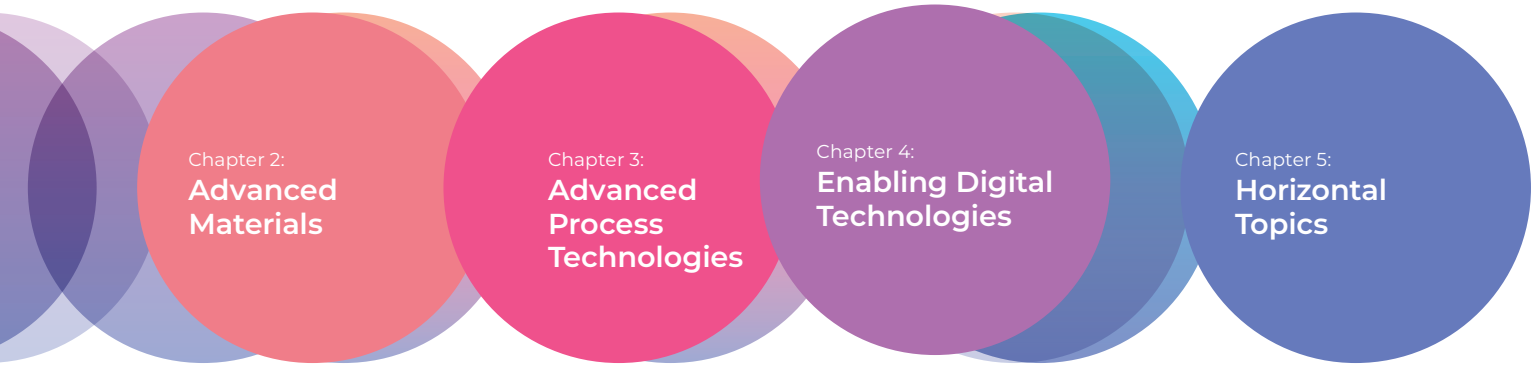
Innovation Fund (2021-2030) aims at creating the right financial incentives for industry to invest in the next generation of technologies needed for the EU's low-carbon transition. SusChem technology priorities closely linked to valorisation of alternative feedstock and/or energy could thereby benefit from the Innovation Fund.

European Structural and Investment Funds (ESIF) (2021-2027) is designed to develop and support actions, related to key EU priorities, through European funds such as the currently available ones: the European Regional Development Fund (ERDF), the European Social Fund (ESF), the Cohesion Fund (CF), the European Agricultural Fund for Rural Development (EAFRD) and the European Maritime and Fisheries Fund (EMFF). As such, many demo projects relevant to SusChem may be built on ESIF.

Eureka is a facilitator of innovation, providing a proven platform for transnational market-oriented RD&I cooperation. It facilitates access to finance for companies involved in topics that are also closely linked to SusChem e.g. Energy, Environment, Information, Medical and Biotechnological Technologies, New materials, Automation, and Transport.

New SusChem SIRA: Navigating Through the Technology Priorities

The SusChem technology priorities are summarised under the following main chapters:



Each chapter starts with an executive summary, moving to selected technology priorities, under each: the context, market and overall expected impact, as well as horizontal challenges are addressed.

For each technology priority, a short assessment against the impact on UN SDGs and a focused summary table on the relevance to Horizon Europe *(agreed HEU text of the draft Council decision, April 15, 2019)* is provided. The SusChem priorities are specifically assessed against HEU Pillar II (clusters and intervention areas) given its thematic approach.

Provided that there are synergies between the three areas of innovation, links across technology priorities are proposed as well ('SusChem pillars – multi KETs' section).

For further defining the scope of each priority, specific RD&I actions are recommended. The actions of the highest priority are elaborated further, including their specific challenges and specific expected impact, with impact examples from EU initiatives and/or projects but also TRL 2030 progression, using application areas as examples.

Horizontal topics with priorities for horizontal impact, being at the core of the SusChem vision, are elaborated in Chapter 5. These complementary topics are essential for the optimal deployment of sustainable chemistry and for maximising its contribution to solving global challenges. More specifically, the following horizontal topics are addressed:

- Sustainability assessment of innovation
- Safe-by-design approach for chemicals and materials
- Building on education and skills capacity in Europe

The following tables connect (Tables 1-3) the three overarching and interconnected challenge areas of focus to SusChem ('Circular Economy and Resource efficiency', 'Low carbon economy', 'Environmental and Human Health') with the technology priorities elaborated in this SusChem SIRA (Chapter 2, 3, 4 and 5).

Circular Economy and Resource Efficiency

Table 1: Circular Economy and Resource Efficiency - SusChem Technology Priorities

FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
MATERIALS DESIGN FOR DURABILITY	• Composites and cellular materials **(2.1)** • 3D-printable materials **(2.2)** • Bio-based materials **(2.3.1, 2.3.2, 2.3.3)** • Additives **(2.4)** • Biocompatible and smart materials **(2.5)** • Materials for electronics, sensors and photovoltaics **(2.6)** • Membranes **(2.7)** • Materials for energy storage **(2.8)** • Coating materials and aerogels **(2.9)** • Laboratory 4.0 – Digital R&D **(4.1.1, 4.1.2, 4.1.3)**
MATERIALS DESIGN FOR RECYCLABILITY	• Composites and cellular materials **(2.1)** • Bio-based materials **(2.3)** • Additives **(2.4)** • Materials for electronics, sensors and photovoltaics **(2.6)** • Membranes **(2.7)** • Materials for energy storage **(2.8)** • Coating materials and aerogels **(2.9)** • Laboratory 4.0 – Digital R&D **(4.1.1, 4.1.2, 4.1.3)** • Data sharing platforms/data security **4.7** • Distributed-ledger technologies **(4.1)**
WASTE AS ALTERNATIVE FEEDSTOCK	• New Reactor & Process design concepts and equipment **(3.1)** • Modular production **(3.2)** • Separation process technologies **(3.3)** • Reactor & Process design concepts for non-conventional energy forms **(3.4.1, 3.4.3)** • Electrochemical and Electrocatalytic processes **(3.5)** • Catalysis **(3.9.2)** • Industrial biotechnology **3.10** • Waste valorisation process technologies **(3.11.1)** • Laboratory 4.0 – Digital R&D **(4.1.3)** • Process analytical technologies **(4.2.1)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **4.3** • Data sharing platforms/data security **4.7** • Coordination and management of connected processes **4.8** • Distributed-ledger technologies **4.9** • Additives for tracking (sorting and separation) **(2.4.1)** • Membranes **(2.7)**

Circular Economy and Resource Efficiency

Table 1: Circular Economy and Resource Efficiency - SusChem Technology Priorities

FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
BIOMASS AS ALTERNATIVE FEEDSTOCK	• New Reactor & Process design concepts and equipment **(3.1.1, 3.1.4)** • Modular production **(3.2)** • Separation process technologies **(3.3)** • Reactor & Process design concepts for non-conventional energy forms **(3.4.1, 3.4.3)** • Catalysis **(3.9.1)** • Industrial biotechnology **3.10** • Laboratory 4.0 – Digital R&D **(4.1.3)** • Process analytical technologies **(4.2.1)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **(4.3)** • Data sharing platforms/data security **(4.7)** • Coordination and management of connected processes **(4.8** • Distributed-ledger technologies **(4.9)** • Bio-based chemicals and materials **(2.3)**
CO_2 /CO AS ALTERNATIVE FEEDSTOCK	• New Reactor & Process design concepts and equipment **(3.1)** • Separation process technologies **(3.3)** • Reactor & Process design concepts for non-conventional energy forms **(3.4.1, 3.4.4)** • Electrochemical and Electrocatalytic processes **(3.5)** • Power-to-Chemicals **(3.8.1, 3.8.2, 3.8.3)** • Catalysis **(3.9.3)** • Industrial biotechnology **(3.10.1, 3.10.2)** • Laboratory 4.0 – Digital R&D **(4.1.3)** • Process analytical technologies **(4.2.1)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **(4.3)** • Data sharing platforms/data security **(4.7)** • Coordination and management of connected processes **(4.8)** • Membranes for gas separation **(2.7.2)**
SUSTAINABLE WATER MANAGEMENT	• Process technologies for advanced water management **(3.12)** • Process analytical technologies **(4.2.1)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **(4.3v** • Advanced (big-) data analytics and artificial intelligence **(4.4.3)** • Coordination and management of connected processes **(4.8)** • Membranes for separation in diluted conditions and water treatment applications **(2.7.1)**

FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
RECOVERY AND REUSE OF CRITICAL RAW MATERIALS AND/OR THEIR SUSTAINABLE REPLACEMENT	• Electrochemical processes **(3.5.2)** • Waste valorisation process technologies **(3.11.2)** • Separation process technologies **(3.3)** • Process technologies for advanced water management **(3.12)** • Process analytical technologies **(4.2.1)** • Distributed-ledger technologies **(4.9)** • Membranes for separation in diluted conditions and water treatment applications **(2.7.1)** • Membranes for organic and inorganic separations (concentrated systems **(2.7.3)** • Materials for energy storage **(2.8.1, 2.8.2, 2.8.3, 2.8.4)**
INDUSTRIAL SYMBIOSIS	Note: Please see above sections on 'Biomass as alternative feedstock', 'CO_2/CO as alternative feedstock', 'Waste as alternative feedstock' and 'Sustainable water management'.
INCREASE VALUE CHAIN COLLABORATION, INFORMING THE CONSUMER AND B2B ON REUSE AND RECYCLABILITY	• Data sharing platforms/data security **(4.7)** • Coordination and management of connected processes **(4.8)** • Distributed-ledger technologies **(4.9)**
SUPPORTING DECISION MAKING, ACCOUNTING FOR CIRCULARITY	• Laboratory 4.0 – Digital R&D **(4.1)** • Advanced (big)-data analytics and artificial intelligence **(4.4)** • Digital support of operators and human-process interfaces **(4.6)** • Coordination and management of connected processes **(4.8)** • Data sharing platforms/data security **(4.7)** - Sustainability assessment innovation **(5.1)** - Safe-by-design for chemicals and materials **(5.2)** - Building on education and skills capacity in Europe **(5.3)**

* For 'Safe-by-design for chemicals & materials', please see Table 3.

Low Carbon Economy

Table 2: Low Carbon Economy - SusChem Technology Priorities

FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
SUSTAINABLE PRODUCTION OF RENEWABLE ELECTRICITY	• Thin film photovoltaics **(2.6.2)** • Multi-junction photovoltaic materials **(2.6.3)** • Materials for wind turbines **(2.1.3)** • Laboratory 4.0 – Digital R&D **(4.1.1, 4.1.2, 4.1.3)**
RENEWABLE ENERGY STORAGE	• Materials for energy storage **(2.7)** • Hydrogen production with a low-carbon footprint **(3.7.1, 3.7.2, 3.7.3)** • Power-to-chemicals process technologies • Catalysis **(3.9.3)** • Laboratory 4.0 – Digital R&D **(4.1.1, 4.1.2, 4.1.3)**
ENERGY EFFICIENCY IN TRANSPORT AND BUILDINGS	• Composites and cellular materials **(2.1)** • Materials for energy storage **(2.7)** • Laboratory 4.0 – Digital R&D **(4.1.1, 4.1.2, 4.1.3)**
ELECTRIFICATION OF CHEMICAL PROCESSES, AND USE OF RENEWABLE ENERGY SOURCES	• New Reactor & Process design concepts and equipment **(3.1.2, 3.1.3)** • Reactor & Process design concepts for non-conventional energy forms **(3.4)** • Electrochemical and Electrocatalytic processes **(3.5)** • Power-to-Chemicals • Hydrogen production with low carbon footprint **(3.7.1, 3.7.2, 3.7.3)** • Power-to-Heat **(3.6)** • Catalysis **(3.9.3)** • Laboratory 4.0 – Digital R&D **(4.1.3)** • Coordination and management of connected processes **(4.8)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **(4.3)** • Advanced (big)-data analytics and artificial intelligence **(4.4)**

FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
INCREASED ENERGY EFFICIENCY OF CHEMICAL PROCESS TECHNOLOGIES	Overarching goal: See full Chapter 3: Advanced Processes and Chapter 4: Enabling Digital Technologies
ENERGY EFFICIENT WATER TREATMENT	• Process technologies for advanced water management **(3.12** • Process analytical technologies **(4.2.1)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **(4.3)** • Advanced (big-) data analytics and artificial intelligence **(4.4.3)** • Coordination and management of connected processes **(4.8)** • Membranes for separation in diluted conditions and water treatment applications **(2.7.1)**
INDUSTRIAL SYMBIOSIS VIA BETTER VALORISATION OF ENERGY STREAMS	• Data sharing platforms/data security **(4.7)** • Coordination and management of connected processes **(4.8)** • New Reactor & Process design concepts and equipment **(3.1)** • Power-to-Heat **(3.6)**
ALTERNATIVE BUSINESS MODELS (SECTOR COUPLING)	• Data sharing platforms/data security **(4.7)** • Coordination and management of connected processes **(4.8.2, 4.8.3)**
SUPPORTING DECISION MAKING	• Laboratory 4.0 – Digital R&D **(4.1)** • Advanced (big)-data analytics and artificial intelligence **(4.4)** • Digital support of operators and human-process interfaces **(4.6)** • Coordination and management of connected processes **(4.8v** • Data sharing platforms/data security **(4.7)** • Sustainability assessment innovation **(5.1)** • Building on Education and skills capacity in Europe **(5.3)**

* Low carbon economy refers to GHGs emissions into the biosphere, and specifically CO_2.

SUSCHEM

Environmental and Human Health

Table 3: Environmental and Human Health - SusChem Technology Priorities

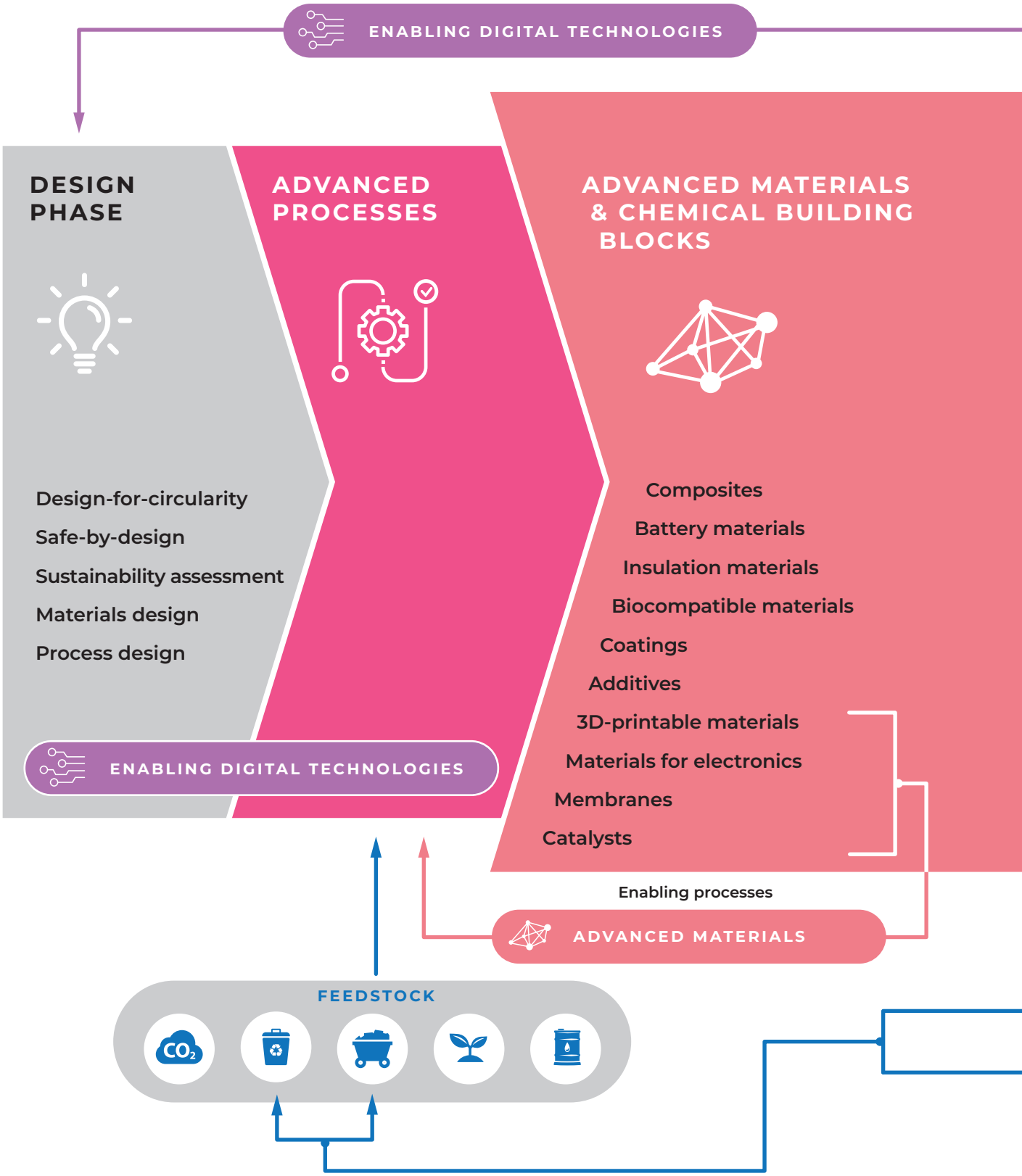
FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
SAFE-BY-DESIGN	• Safe-by-design for materials and chemicals (functionality approach, methodologies, data) **(5.2)** • Laboratory 4.0 – Digital R&D **(4.1)** • Data sharing platforms/data security **(4.7)** • Distributed-ledger technologies **(4.9)** • Process and plant design*
IMPROVE SAFETY OF OPERATIONS	• Laboratory 4.0 – Digital R&D **(4.1)** • Process analytical technologies **(4.2)** • Cognitive plants: (real-time) process simulation, monitoring, control and optimisation **(4.3)** • Advanced (big)-data analytics and artificial intelligence **(4.4)** • Predictive maintenance **(4.5)** • Digital support of operators and human-process interfaces **(4.6)** • Data sharing platforms/data security **(4.7)** • Process and plant design*
ZERO-WASTE DISCHARGE PROCESSES	See contribution from priorities in the 'Circular Economy and Resource Efficiency' table
ZERO-LIQUID DISCHARGE PROCESSES	• Process technologies for advanced water management **(3.12** • Process analytical technologies **(4.2.1)** • Advanced (big)-data analytics and artificial intelligence **(4.4.3)** • Membranes for separation in diluted conditions and water treatment applications **(2.7.1)**
TECHNOLOGIES FOR REDUCTION OF GHGs EMISSIONS	See contribution from priorities in the 'Low Carbon Economy' table, complemented by technology priorities in the 'Circular Economy and Resource Efficiency' table
TECHNOLOGIES FOR REDUCING INDUSTRIAL EMISSIONS	• Sustainability assessment innovation **(5.1)** • Safe-by-design for chemicals and materials **(5.2)**

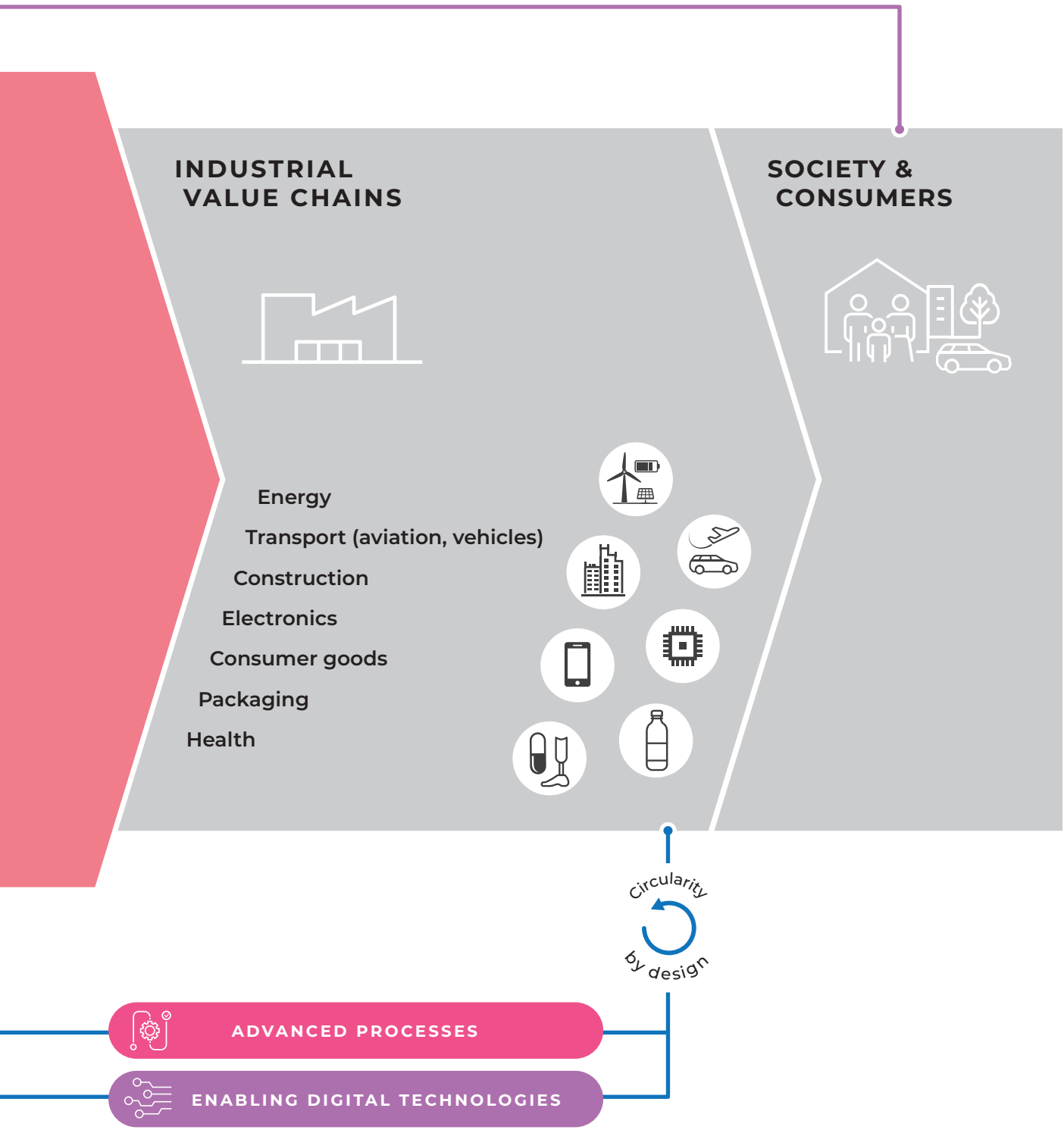
FOCUS AREAS	SUSCHEM TECHNOLOGY PRIORITIES (KEY EXAMPLES)
SUSTAINABLE SOURCING OF RAW MATERIALS	See contribution from priorities in the 'Circular Economy and Resource Efficiency' table • Sustainability assessment innovation **(5.1)**
INCREASING TRANSPARENCY OF PRODUCTS WITHIN VALUE CHAINS THROUGH DIGITAL TECHNOLOGIES	• Data sharing platforms/data security **(4.7)** • Distributed-ledger technologies **(4.9)**
ALTERNATIVE FOOD TECHNOLOGIES	• Biotech solutions to upgrade plant-based raw materials as high-quality meat replacements **(3.10.3.1)** • Non-lignocellulosic bio-based products **(2.3.3)** • Laboratory 4.0 – Digital R&D **(4.1)**
NOVEL THERAPEUTICS AND PERSONALISED MEDICINE	• Production and metrology of specialty carbohydrates and lipids **(3.10.3.1)** • Biocompatible and smart materials **(2.5)** • Laboratory 4.0 – Digital R&D **(4.1)**
SUSTAINABLE AGRICULTURE, FORESTRY AND SOIL HEALTH RELATED TECHNOLOGIES	• Biotech solutions to upgrade plant-based raw materials as high-quality meat replacements **(3.10.3.1)** • Enhancing positively the health of the environment through novel products for sustainable agriculture, forestry and ocean harvesting **(3.10.3.4)** • Biodegradable and/or compostable polymers **(2.2.4)** • Laboratory 4.0 – Digital R&D **(4.1)**
MATERIALS FOR HEALTH APPLICATIONS	• Biocompatible and smart materials **(2.5)** • 3D-printable materials **(2.2)** • Laboratory 4.0 – Digital R&D **(4.1)**

*Note: Process safety remains an inherent and overarching element of process design for chemical and biotech processes

2 ADVANCED MATERIALS

Advanced materials as solutions for other industrial value chains




INDUSTRIAL VALUE CHAINS
SOCIETY & CONSUMERS
Energy
Transport (aviation, vehicles)
Construction
Electronics
Consumer goods
Packaging
Health
Circularity by design
ADVANCED PROCESSES
ENABLING DIGITAL TECHNOLOGIES

SusChem Technology Priorities: Advanced Materials

'Advanced materials' are the basis for innovation in a wide range of industries such as transport, food, consumer goods, electronics, energy, health, construction, computing, telecommunications, and water as well as waste management and recycling, with the potential to enable these and other interlinked industries to achieve sustainable growth. Advanced materials can make buildings and infrastructures more durable and energy efficient; they make vehicles lighter and safer; and they make high-performance products and devices for health and wellbeing. Innovation enables new functionalities and properties resulting in new products/applications or enhancements of existing products. This can thereby address new market applications to meet end-user demands, new value chains as well as the successful integration of alternative carbon feedstock such as CO, waste and biomass.

Advanced materials' wide outreach contributes to European industrial competitiveness, environmental performance and the circular economy, by improving energy and resource efficiency as well as via circularity-by-design. In the context of transitioning to a circular economy, some key challenges include the sustainable recycling of materials, which goes beyond materials innovation and includes synergy with advanced processes and the opportunities that digital technologies can offer.

Horizontal priorities:

- Materials innovation for improvements in functionality and/or durability, whilst increasing circularity-by-design (sorting & separation, recycling), supported with Advanced Processes **(Chapter 3)** and enabling Digital Technologies **(Chapter 4)**;
- Improved materials design, processing and characterisation, enabled by digital technologies **(Chapter 4)**.

Summary of key priorities for advanced materials to be addressed:

- Design and further development of catalysts for advanced processes **(Chapter 3, 3.9)**;
- Develop **composites** with high-performance under demanding conditions;
- **Coatings** performing in highly demanding environments;
- Improving **batteries/energy storage** performance;
- Materials design for circularity (e.g. **circularity-by-design** for composites);
- **Additives** for improved materials **tracking, separation** and **recycling**;
- Increase separation selectivity and energy performance of **membranes**;
- Further developing sustainable **bio-based chemicals and materials**;
- Improve materials functionality to further advance **3D-printing**;
- Design new **smart materials** and **multi-materials**, with emphasis on new functionalities such as photonic, conductivity, self-healing, and stimuli-responsive properties;
- Further development of **bio-compatibility of materials** for a wider uptake.

Impact of Advanced Materials innovation – UN SDGs

'Industry Innovation and Infrastructure', via sustainable materials, allowing for environmentally sound technologies;

'Responsible consumption and production' by creating circular materials, materials from alternative carbon feedstock and materials for separation technologies that contribute to reduce waste generation through prevention, reduction, recycling and reuse;

'Climate action', through materials that can be applied to enable energy efficiency and lower GHGs emissions;

'Good Health and Well Being', by developing materials that contribute to improve human health;

'Clean water and sanitation', with materials that can be used for water treatment;

'Affordable and Clean Energy', via indirect improvements in energy efficiency and increasing the share of renewable energy;

'Decent work and Economic Growth', by achieving higher levels of economic productivity through technological upgrading and innovation in materials;

'Sustainable cities and communities', by providing materials for energy efficient transport and buildings.

Advanced materials innovation – relevance to Horizon Europe

Advanced materials innovation presents a major contribution to the long-term European policy goals and national priorities. Innovation in materials spans from low to high TRLs, with contributions from academia and industry, thereby linking with Horizon Europe Pillar 1 ('Excellent Science'), Pillar 2 ('Global challenges and European industrial competitiveness') and Pillar 3. ('Innovative Europe'). Given the thematic approach of Pillar 2, the high relevance on the Horizon Europe clusters and areas of intervention is further elaborated (**Table 4**).

Table 4: Relevance of SusChem Priorities on Advanced Materials with Horizon Europe

Horizon Europe

Pillar 2: Global Challenges and European Industrial Competitiveness

Clusters and Intervention areas

CLUSTER 1: Health	1.1 Health throughout the life course
	1.2 Environmental and social health determinants
	1.3 Non-communicable and rare diseases
	1.4 Infectious diseases, including poverty-related and neglected diseases
	1.5 Tools, technologies, and digital solutions for health & care, including personalised medicine
	1.6 Healthcare systems
CLUSTER 4: Digital, Industry and Space	4.1 Manufacturing technologies
	4.2 Key Digital technologies
	4.3 Emerging enabling technologies
	4.4 Advanced Materials
	4.5 AI and Robotics
	4.6 Next generation internet
	4.7 Advanced Computing and Big Data
	4.8 Circular Industries
	4.9 Low-carbon and Clean Industries
	4.10 Space including Earth observation
CLUSTER 5: Climate, Energy and Mobility	5.1 Climate Science and solutions
	5.2 Energy supply
	5.3 Energy grids
	5.4 Buildings and Industrial facilities in energy transition
	5.5 Communities and cities
	5.6 Industrial competitiveness in transport
	5.7 Clean, safe and accessible transport and mobility
	5.8 Smart mobility
	5.9 Energy storage
CLUSTER 6: Food, Bioeconomy, Natural Resources, Agriculture and the Environment	6.1 Environmental Observation
	6.2 Biodiversity and natural resources
	6.3 Agriculture, Forestry and rural areas
	6.4 Seas, Oceans and inland waters
	6.5 Food systems
	6.6 Bio-based innovation systems in the EU Bioeconomy
	6.7 Circular systems

SusChem priorities: ADVANCED MATERIALS

Composites and cellular materials (lightweight, insulation properties)	3D-printable materials	Bio-based chemicals and materials	Additives	Biocompatible and smart materials	Materials for electronics	Membranes	Materials for energy storage	Coating materials and aerogels
	●			●		●		
	●			●	●			
●	●	●	●	●	●	●	●	●
					●			
				●	●			
●	●	●	●	●	●	●	●	●
					●		●	
●	●	●	●		●	●	●	●
						●		
●							●	
●		●			●	●	●	
●	●	●				●	●	●
●	●	●	●		●	●	●	●
●		●			●		●	●
							●	
					●			
						●	●	
		●				●		
		●						
		●	●			●		●
	●	●	●	●				
●	●	●	●		●	●	●	●

2.1 Composites and Cellular Materials (Lightweight, Insulation Properties)

Context: Lightweight and insulation are indispensable features in transport (aeronautics, automotive) and construction to increase energy efficiency and to reach target greenhouse gas (GHG) emissions by 2050.[7] For instance, a reduction of 27.5% on average fleet weight could translate to a reduction of 40% in CO_2 emissions[8] only in the transport sector, which contributes 27% to total EU greenhouse gas emissions. Enhanced functionalities, durability and recyclability are the main driving factors to reach market uptake of composites and cellular materials in increasingly demanding applications.

Market, overall expected impact: The EU fibre-reinforced composites market accounted for 1.2 million tons in 2018, mainly for aerospace (36%), automotive (24%) and wind energy (13%) sectors.[9] Wind energy accounts for 18.8% of the EU's total installed power generation capacity.[10] Lightweight foams are increasingly used in building and construction, packaging, furniture and transport applications, making recyclability crucial. Most composite materials used in these applications are still landfilled or incinerated, and downcycled into fillers, for example in cement co-processing. Process technologies like mechanical recycling, or solvolysis/chemical recycling are alternatives for the valorisation of waste composite materials while such processes could be enhanced by circularity-by-design of materials.

Composites and cellular materials address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Manufacturing technologies' (4.1), 'Advanced Materials' 4.4, 'Circular industries' 4.8, 'Space including Earth observation' (4.10), 'Energy supply' 5.2, 'Buildings and industrial facilities in energy transition' (5.4), 'Communities and cities' (5.5), 'Industrial competitiveness in transport' (5.6) and 'Circular systems' (6.7), mainly by the following factors:

- **Performance and durability of critical and structural parts** leads to increased system efficiency, even in demanding applications (e.g. transportation, construction, electricity production) and severe conditions (e.g. resistance to corrosion, fire resistance and dimensional stability);
- **Energy efficiency and CO_2 emissions reduction in buildings, transport and infrastructure** derived mainly from the use of lightweight foams and materials for thermal insulation;
- **Circularity-by-design** contributing to circular economy and circular industries.

Horizontal challenges:

- Implementation of circular approaches and eco-design principles to facilitate recovery and recyclability of composites and cellular materials (e.g. fibre-reinforced composites, and foams).

SUSCHEM PILLARS – MULTI-KETS:

Contributions of innovation in **Advanced Processes (Chapter 3)** include: 'Tolerant and intensified reactors and processes – tolerance to feedstock variability' (3.1.1), 'Enabling waste valorisation via catalysis' (3.9.2), 'Separation process technologies' (3.3), and 'Chemical recycling of plastics waste' (3.11.1).

The design and production of composites and cellular materials will be supported by **Enabling Digital Technologies (Chapter 4)**: 'Materials and molecules design: modelling and simulation developments' (4.1.1), 'Materials and formulations design– integration with process design' (4.1.2), 'Distributed-ledger technologies' 4.9, and 'Enabling transparent supply chains' (4.9.1).

Within **Advanced Materials** the relevant topics include: 'Additives' (2.4) and 'Coating materials and aerogels' (2.9).

RD&I Actions

2.1.1 Fibre-reinforced (FRP) plastics: Performance and durability improvements

Context: The long-term performance and durability of fibre-reinforced plastics under harsh environmental conditions, still represents a critical issue.

Specific challenges:

- Functional additives designed for required efficiency and prolonged life (e.g. improve corrosion or fire resistance);
- Increase materials' mechanical performance, for high-demanding or structural applications (e.g. use of nanofibres);
- Approaches to simulate the ageing behaviour of FRP plastics in severe and harsh conditions and implement with materials design.

Specific expected impact: Fibre-reinforced plastics enhanced durability and lifetime will have a positive impact for industries where circularity principles are in development: aerospace, infrastructure and renewable energy.

IMPACT EXAMPLES :

Example 1: Self- sensing, self-de-icing, self-curing and self-healing lightweight composite parts for the aeronautic and automotive sector, incorporating conductive nanomaterials like multi-walled carbon nanotubes and graphite. The aim is to increase consumer safety, component lifespan, and performance, while reducing maintenance and manufacturing costs and greenhouse gas emissions. The development of these components can lead to up to 90 % energy reduction and up to 60 % of the total manufacturing time in aeronautics.[11]

Example 2: Development of semi-industrial scale pre-impregnation process to obtain Space Qualified Intermediate Modulus and High Modulus Prepregs from European-based carbon fibres (CF) for launchers and satellite applications. The aim is to create the capacity in Europe to produce specialty CF products, contributing to improve Europe's worldwide competitiveness in the field of high-performance Carbon Fibre Reinforced Polymer (CFRP) structures.[12]

TRL(now) & TRL(2030): Technologies implying the use of nanofibres, as well as the use of functional additives with prolonged life in severe conditions are currently at TRL 2-4, although some specific applications, such as fire-resistance composites, are at TRLs of 7-8. By 2030, demonstration activities need to be set-up to achieve a TRL 6-8.

2.1.2 Composite resins. Improving recyclability-by-design

Context: Today, most long-fibre or reinforced polymeric composites rely on crosslinked polymers as the matrix resin, while the remainder are based on a thermoplastic matrix. To increase the recyclability of composite resins, the first phase of material formulation and design need to be addressed to fit the recycling technologies that are currently available.

Specific challenges:

- Even though recycling of crosslinked resins carrying polar moieties may be well accessible by solvolysis, this is much more difficult with epoxy resins and other high-performance materials like polyimides. The resin systems will need to be modified for circularity to provide for an efficient chemical recycling option. This should be done without sacrificing processing properties, mechanical strength and/or resistance to humidity.

Specific expected impact: Composite resins are used in aerospace, automotive, construction/infrastructure, electric/electronic applications as well as sport goods. The growing use of composites creates a high demand for improving circularity-by-design for resins, ultimately impacting the EU Circular Economy Strategy.

IMPACT EXAMPLES :

Example 1: Bio-based epoxy resins that are repairable by applying heat and pressure, can be reprocessed to create parts and are recyclable to produce short-fibre reinforced parts. Circularity-by-design is applied by incorporating the concepts of bio-based, repairable, re-processable and recyclable into the material and part design.[13]

Example 2: New circular models including the concepts of reuse, repair, refurbish and recovery for composite products in the furniture, automotive and building sectors. Life-cycle Assessment (LCA) of prototypes show resource reduction of at least 50 %.[14]

TRL(now) & TRL(2030): Technologies involving the development of novel recyclable resins are currently at TRL 2-4; albeit with some exceptions. TRL 6-8 would be expected to be reached by 2030, by innovation actions to prove the economic feasibility.

2.1.3 Materials for wind turbines: Circularity-by-design

Context: Most rotor blades in operation today rely on epoxy resin formulations as the matrix material. Epoxy resins provide ease of processing, high mechanical strength and chemical resistance, but are less suitable for recycling. Waste composites from rotor blades are treated today at commercial scale through cement co-processing, where cement raw materials are partially replaced by the composite's glass fibres as filler, while

the organic fraction replaces coal as a fuel. Chemical recycling and mechanical recycling can be enhanced by circularity-by-design of materials for wind turbines.

Specific challenges:

- Modification of epoxy resins systems to make them suitable for chemical recycling, without sacrificing processing properties (e.g. viscosity, curing conditions), mechanical strength and chemical resistance;
- Developments on other recyclable resin matrices to replace epoxy resins.

Specific expected impact: Considering that a 5 MW wind turbine produces more than 50 tonnes of plastic composite waste from the blades alone, it is estimated that by 2050, 39.8 million tonnes of material from the global wind industry will await disposal, so setting-up strategies for circularity-by-design becomes key.

IMPACT EXAMPLES :

Example 1: Green technology for the recycling of wind turbine blades after their end of life to obtain high quality fibres, energy and fuels.[15] The technology developed allows for the recovery of fibres in reinforced composites (glass or carbon) with different kinds of resins (mainly epoxy and phenolic).

Example 2: Liquid thermoplastic resin suitable for the manufacture of composite parts. The resin provides short setting times at ambient temperature and shows compatibility with technologies for transforming thermosetting resins with the added advantage of recyclability. Besides its high contribution to wind turbines circularity (a prototype 25 metre wind turbine blade has been produced), multiple sectors of application are envisaged such as automotive, construction and sports.[16]

TRL(now) & TRL(2030): Technologies based on the development of novel epoxy resin systems and alternative materials are currently at TRL 2-4. A TRL 6-8 would be expected to be reached by 2030 by the development of innovation actions to further implement those novel material systems into relevant environments.

2.1.4 Lightweight foams: Circularity-by-design, weight reduction and new applications

Context: Packaging and automotive industries rely on foams with good impact resistance allowing low transportation costs and aiming at GHG emissions reduction and enhanced energy efficiency. Lightweight foams with short lifetime, such as packaging and consumer products, lead to excessive amounts of unrecycled waste. Lightweight foams are also used in the building and construction sectors for insulation, flooring, pipes, wires and cables. Furniture is also a large segment with applications such as carpets, mattress padding, fibres, and cushions.

Specific challenges:

- The separation systems of current polymer foams need to be improved and new materials with easier recycling properties need to be developed;
- Achieve significant weight reduction while maintaining structural/mechanical properties;
- Expanding the applications of lightweight foams to new fields by additional functional properties. These include open or closed-cell foams enabling filtering, sensing, or materials with novel mechanical or thermal properties. Alternative lightweight foams based on bio-based polymers could be further explored.

2.1.5 Novel thermoplastics for composites

Context: Recycling thermoset fibre-reinforced plastic parts is challenging with low yields, in particular for the matrix. Additionally, fibres are significantly degraded upon recycling, resulting in downcycling. The recycled material properties can further deteriorate due to chemical incompatibility, possible presence of fillers, and different viscosity ratios. Thermoplastic resin systems have been considered in large-scale composite parts but have yet to be upscaled. The use of these resins versus their thermosetting counterparts can introduce cost savings due to non-heated tools for curing and shorter manufacturing cycle times. Recycling of thermoplastic fibre composites via dissolution into their constituent parts is commercially feasible, while this is not possible with thermoset composites. There is an increasing trend toward using thermoplastic resins in long fibre composites.

Specific challenges:

- Development of reinforced thermoplastics with controlled dispersion and orientation of the fibres, maintaining the final material for high demanding applications (e.g. rotor blades). An additional critical point is to achieve simplifications in the current production processes.

2.2 3D-Printable Materials

Context: 3D-printing techniques (also known as additive manufacturing) to produce objects started mainly using plastic materials, but metal, ceramics, glass, paper, concrete, food, and even living cells are nowadays also under development.[17] '3D-printable materials' remains a fast-developing area, covering 3D-printed polymers, composites, or multi-materials, as well as precursors for one-step polymerisation. They have applications in medical devices, pharma (i.e. personalised medicine), bio-printing, food, transport or construction.

Market, overall expected impact: Additive manufacturing (AM) is estimated to generate economic revenues of $35.6 billion by 2024,[18] for a wide range of applications, including transport, energy storage and production, buildings and infrastructure, health and wellbeing, consumer goods, industry applications, or packaging.[19] The biomedical market represents more than 11 % of the AM market and it is considered a key driver for its future growth.[20]

3D-printable materials address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Health throughout the life course' (1.1), 'Tools technologies and digital solutions for health and care, including personalised medicine' (1.5), 'Manufacturing technologies' (4.1), 'Advanced Materials' 4.4, 'Circular industries' 4.8, 'Buildings and industrial facilities in energy transition' (5.4), 'Communities and cities' (5.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular systems' (6.7), mainly by the following factors:

- **The cost- and resource- effective production of complex 3D-printed objects** as well as their **mass-customisation, rapid manufacturing and prototyping;**
- **The valorisation of alternative feedstock** by i.e. using polymer matrixes derived from waste or from bio-polymers for 3D-printing.

Horizontal challenges:

- Development of materials, including from waste and biomass, to meet end-use performance criteria for a wide range of applications whilst being adapted/adaptable to 3D-printing process technologies;
- Integration of multiple materials, allowing the production of more complex objects;
- Application of LCA studies of additive manufacturing vs. conventional manufacturing and optimisation of process parameters for materials production.[21]

SUSCHEM PILLARS – MULTI-KETS:

Contributions of innovation in **Advanced Processes (Chapter 3)** include: 'Microreactor systems' (3.1.5), '3D-printing of reactors' (3.1.12), and 'Catalysis' (3.9).

The design and production of 3D-printable materials will be supported by **Enabling Digital Technologies (Chapter 4)**: 'Materials and molecules design: modelling and simulation developments' (4.1.1), 'Materials and formulations design– integration with process design' (4.1.2) and 'Inline Process monitoring for material deposition' (4.4.2).

Within **Advanced Materials** the relevant topics include: 'Composites and cellular materials' (2.1), 'Bio-based materials' (2.3), 'Additives' (2.4), 'Biocompatible and smart materials' (2.5), and 'Materials for electronics' (2.6).

RD&I Actions

2.2.1 Functional bio-based 3D-printed polymers

Context: Bio-based polymers and bio-polymers (e.g. cellulose) can be used as an alternative carbon-source for the synthesis of 3D-printable materials, with circularity by-feedstock as their main added attribute. Such materials can have a wide range of applications in construction, automotive, or health. Production of 3D-printable bio-based polymers (drop-in and dedicated structures) with the appropriate thermal stability is necessary. Polyethylene furanoate (PEF) and Polycarbonate (PC) specifically show promise in expanding the current bio-polymer use in 3D-printing, with PEF and PC currently targeted at consumer products. Chemical, biological, and mechanical properties and especially water stability and control of degradation of the final product need to be enhanced before achieving the full potential of bio-based polymers for 3D-printing.[22]

Specific challenges:

- Further develop polyamides (PAs) from biological sources since properties can vary greatly;
- Improve performance of 3D-printed bio-based materials for applications where high thermal stability is required, such as application where today polycarbonates (PC) are used.

Specific expected impact: Potential to reduce the production process carbon footprint by valorising alternative carbon feedstock and contribute to the European Bioeconomy strategy.

IMPACT EXAMPLES:

Example 1: Biopolymers with advanced functionalities for building and automotive parts processed through fused filament fabrication (3D-printing), derived from food waste and agro-waste (lignocellulosic) feedstock.[23]

Example 2: Polyethylene furanoate (PEF) offers promising opportunities for 3D-printing due to its enhanced thermal and mechanical properties over other bio-based polymers. For applications in which temperature stability is the key metric, polycarbonate (PC) stands out among bio-based thermoplastics.[24] Applications extend to consumer products and automotive components.

TRL(now) & TRL(2030): The development of bio-based 3D-printed polymers is at a relatively low TRL (2-4). Fundamental research is at a lower TRL (1-5) on exploring new bio-based polymers and their properties and stability for 3D-printing needs to be achieved by 2030.

2.2.2 Dual/multi-material 3D-printing, robust to raw materials variability

Context: Printing objects using two or several materials at once is the key capability of 3D-printing that could leverage its potential. By integrating several materials in 3D-printing, the need for assembling, post-processing stages (e.g. colouring) can be eliminated. Furthermore, dual/multi-material 3D-printing allows more efficient design of multifunctional and more complex objects and helps to reduce not only manufacturing time but also cost.[25]

Specific challenge: Dual/multi-material 3D-printing complexity due to the different material characteristics requires process and/or materials design to be addressed.

Specific expected impact: Achieve increased complexity of objects being produced in a sustainable manner. Further, these technologies may lead to new business models.

IMPACT EXAMPLES:

Example 1: Development of 3D-printing technology capable of printing truly multi-material parts to be able to combine metals, polymers and ceramics, producing more complex materials by enabling unique material combinations.[26]

Example 2: Development of a multi-material 3D-printing technology to fabricate micro-structured detection devices with the ability to perform all steps of chemical analysis in an automated fashion in one continuous biochemical detection system.[27]

TRL(now) & TRL(2030): Dual/multi-material 3D-printing has a relatively low TRL (2-3). Fundamental research exploring multi-materials: composite printing through multiple printer heads to print blended and/or layered composites[28] as well as demonstration activities need to be considered to achieve TRL 7-8 by 2030.

2.2.3 One-step polymerisation and 3D-printing

Context: Two-Photon Polymerisation (2PP) is a technology suited for the fabrication of nearly arbitrary 3D micro- and macro- structures rendered possible by tightly focusing femtosecond laser pulses. 2PP offers huge potential in the fabrication of innovative microstructures and complex topographies, particularly non-spherical or free-form designs. The objective is to identify suitable monomers and potentially also improve the recyclability of the 3D-printed objects.

Specific challenges:

- Polymer precursors suitable for 2PP together with computer-aided design/computer-aided manufacturing (CAD-CAM) aiming at tuneable mechanical properties.

Specific expected impact: One-step polymerisation will allow more efficient ways to produce complex objects not easily obtainable by the established techniques (injection moulding, extrusion, etc.) for a wide scope of applications (photonics, health, consumer goods, automotive, aerospace).

IMPACT EXAMPLES :

Example 1: 3D-printed realistic model of the brain tumour microenvironment with its associated blood neurovascular structures: Artificial components of a biomimetic dynamic 3D-system scale of physiological parameters fabricated through two-photon polymerisation (2PP). The manufacturing approach allows the fast fabrication of low-cost structures with nanometre resolution and great levels of reproducibility/accuracy.[29]

TRL(now) & TRL(2030): The state of the art for photopolymerisation technologies and respective materials are currently at a high TRL. Emerging technologies such as 2PP have a low TRL as this is still very much limited to lab research, further RD&I needs to be undertaken to achieve a TRL 7 by 2030.

2.2.4 3D-printable materials for medical and pharma applications

Context: 3D-printable materials applicable for medical devices, implants, or surgical instruments can be personalised and potentially further incorporate functionalities that can enable sensing. 3D-printed ceramics can be applied in porous scaffolds for tissue engineering and wound healing, with suitable mechanical properties and bio-compatibility. 3D-printed materials can also be used in the pharma industry for personalised medicine (e.g. personalised dosages and/or drugs mixtures in tablets).

Specific challenges:

- Regulatory barriers and long validation and assessment periods. 3D-printable materials for health applications require in vitro and in vivo testing, increasing scale up costs and prolonging time-to-market;
- Production scaling issues, cost, reproducibility and quality control are particular challenges for the use of 3D-printing for personalised medicine.

2.3 Bio-based Chemicals and Materials

Context: Bio-based materials are derived from biomass sources (e.g. starch, forestry side streams, agriculture crops and residues, aquatic biomass, food processing residues, municipal organic waste) and can be used to produce platform chemicals, fuels, solvents, polymers and composites. Furthermore, some of the bio-based polymers can be made biodegradable or compostable, based on standards and driven by applications such as food packaging. Bio-based products have the potential of additional functionalities as well as improved environmental performance, further contributing to reducing the dependence on fossil fuels and overall feedstock diversification in the chemical sector. The overall environmental performance and CO_2 footprint over fossil-based equivalents, must always be evaluated in a life-cycle assessment (LCA), considering appropriate system boundaries.

Market, overall expected impact: The overall biomass use in the EU has grown by around 8.5% over 2010-2015. Most of the increase was due to rising demand for bioenergy (+67 Mt, 32% growth), followed by increased demand for bio-based materials (+15 Mt, 5,6% growth). A recent Joint Research Centre (JRC) study has determined the top 10 chemical product categories and their application markets within the EU bio-based products sector.[30] The predicted EU-based production and growth in 2025 included platform chemicals (353 kt/y , Compound Annual Growth Rate (CAGR) 10%), adhesives (462 kt/y, CAGR 10%), surfactants (1 974 kt/y, CAGR 4%), paints, coatings, inks and dyes (1 151 kt/y, CAGR 2%), solvents (80 kt/y, CAGR 1%), polymers for plastics (353 kt/y, CAGR 4%), plasticisers (83 kt/y, CAGR 3%), man-made fibers (738 kt/y, CAGR 3%), lubricants (254 kt/y, CAGR 1%), and cosmetics & personal care products (687 kt/y, CAGR 3%). Regarding bio-based polymers (e.g. bio-based Polyethylene terephthalate (PET), Polyethylene (PE), Polylactic acid (PLA) and starch), packaging is the main application, with some (e.g. PLA) being biodegradable. In addition, bio-based polyurethane (PU) finds applications in construction, transport, consumer goods, and coatings.

Improving the use of existing feedstock sources towards the production of materials and other high-value products is still required, yet new biomass feedstock sources should be further valorised. In the context of expanding the choices and availability of biomass sources, lignocellulosic and aquatic biomass have been regarded as a valuable feedstock for biorefining due

to their high productivity and potential for avoiding competition with arable land. Overall, we need to foster the sustainable use of biomass in both existing and new value chains, with high-value products to ensure the sustainable development of future biorefineries.

Bio-based chemicals and materials address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Manufacturing technologies' (4.1), 'Advanced materials' 4.4, 'Circular Industries' 4.8, 'Low Carbon and Clean Industries' 4.9, 'Buildings and industrial facilities in energy transition' (5.4), 'Communities and cities' (5.5), 'industrial competitiveness in transport' (5.6), 'Agriculture, forestry and rural areas' (6.3), 'Seas, oceans and inland waters' (6.4), 'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular systems' (6.7) mainly by:

- **The sustainable use of biomass feedstock for drop-in and/or dedicated chemical and material structures** with an impact on the bulk and fine chemicals industry and on sectors such as consumer goods, packaging, transport, buildings and infrastructure and an overall high potential for life cycle environmental performance improvements;
- **The valorisation of biomass to produce chemicals and materials** contributes to the circular economy approach, with the food, agriculture and aquaculture industries also being impacted by the recovery of biomass as feedstock.

Horizontal challenges:

- Management of materials resources, feedstock availability and land use;
- Higher cost of production in many product categories, driven by high feedstock prices and/or due to technologies that have not yet been optimised;
- Biomass feedstock composition variability increases the complexity of upstream and downstream processes with especially challenging purification steps;
- Comprehensive circular strategies to design bio-based materials for recyclability;
- Biodegradable materials provide unique properties in specific applications such as the collection and treatment of food waste, albeit environmental claims regarding biodegradability or compostability should comply with appropriate standards. Harmonised rules for defining and labelling compostable and biodegradable plastics are being created at European level. [31]

SUSCHEM PILLARS – MULTI-KETS:

Contributions of innovation in **Advanced Processes (Chapter 3)** include: 'Tolerant and Intensified Reactors and Processes – tolerance to feedstock variability' (3.1.1), 'Enhancing biomass catalytic valorisation' (3.9.1), 'Separation process technologies' (3.3), 'Modular production' (3.2), 'Advanced processes; Industrial biotechnology' 3.10, and 'Waste valorisation process technologies' 3.11.

The design and production of bio-based chemicals and materials will be supported by **Enabling Digital Technologies (Chapter 4)**: 'Materials and molecules design: modelling and simulation developments' (4.1.1), 'Materials and formulations design– integration with process design' (4.1.2), 'Coordination and management of processes/plants/sites towards industrial symbiosis' 4.3, 'Process analytical technologies (PAT)' 4.4, 'Distributed-ledger technologies' 4.9 and 'Enabling transparent supply chains' (4.9.1).

Within **Advanced Materials** the relevant topics include: 'Composites and cellular materials' (2.1), '3D- printable materials' (2.2) and 'Additives' (2.4).

RD&I Actions

2.3.1 Cellulose and hemicellulose-derived products

Context: Cellulose and hemicellulose are environmentally benign, biodegradable, recyclable, and renewable bio-polymers. Cellulose represents about 1.5 x 10 tons of annual production.[32] Several technologies, based on chemical, biotechnological and physical processes or a combination thereof, have shown the potential to convert biomass into cellulose. Sugars from cellulose (glucose) and hemicellulose (xylose, mannose, galactose, arabinose and rhamnose) can be fermented into biofuels or other high-value products to increase the viability and profitability of a biorefinery. Derivatives of cellulose, nano- and micro- cellulose and cellulose-based fibres have a wide range of applications ranging from pharmaceuticals, cosmetics, medical, agricultural, food, textile, construction and buildings to the paper & pulp sectors.

Specific challenges:

- Lignocellulosic biomass pre-treatment and separation of cellulose from other bio-polymers (lignin and hemicellulose) prior to hydrolysis;
- Cost effective scaled-up production of bacterial cellulose;
- Improving on harsh hydrolysis process conditions to break down cellulose into oligosaccharides and glucose;
- Selective glucose conversion to obtain a range of furanics and their subsequent conversion to several high value products (drop-in or dedicated structures);
- Use of currently underutilised biomass and convert C5 and C6 sugars into biofuels (process efficiency improvements and enzymatic catalysis optimisation);
- Stability of micro- and nano-cellulose structures along the production process;
- Formulation of micro- and nano-cellulose for application-oriented performance (stability, durability, mechanical and physical properties);
- Chemical functionalisation, solubilisation of cellulose derivatives (application-oriented).

Specific expected impact: Cellulose and hemicellulose-derived products are expected to have impact on feedstock diversification. Chemical building blocks derived from cellulose and hemicellulose contribute to high value biorefinery products. Furthermore, given the unique structural attributes (i.e. crystalline, amorphous structures, polymer chain length) and chemical functionalities that they can provide, there is an existing and growing demand for high-value applications such as thickeners, excipients and stabilisers, with applications in various sectors. In addition, the growing demand for cellulose and hemicellulose, not only for chemicals but also for biofuels, will continue to contribute in enhancing the upscaling of integrated biorefineries.

IMPACT EXAMPLES:

Example 1: Aerobic fermentation, starting from fruit/vegetable waste, to produce a bio-based nanomaterial, combining the positive attributes of cellulose, with properties such as extraordinary mechanical strength, aiming at the €0.9bn global market for flexible packaging for the food industry with a market share of 2.4%.[33]

Example 2: Bio-based, biodegradable and compostable food packaging from multilayer PLA structure, reinforced with cellulose nanocrystals, able to improve the barrier properties 100 times compared to other bio-based packaging, allowing 300% lengthened shelf life of foods contained therein.[34]

Example 3: Commercial-scale flagship plant to produce cellulosic ethanol from agricultural residues. The plant annual capacity of 50,000 tons of cellulosic ethanol will ensure a highly sustainable process that uses co-products for renewable energy production, reduces GHG emissions and thus accelerates the low carbon economy transition within the transport sector.[35]

TRL(now) & TRL(2030): The various levels of development of the technologies to produce fuels, chemicals and materials is highly impacted by the feedstock used in the respective process as well as the application. This implies a wide TRL range.[36] It is recommended to continue demonstrating the technical and commercial viability of cellulose and hemicellulose-derived products through innovation and demonstration actions by 2030.

2.3.2 Lignin-derived products

Context: Lignin is the second most abundant polymer on earth, making up to 10–25% of plant biomass. Chemically, lignin is a complex polymer assembled from aromatic building blocks that could be regarded as an important renewable source in the production of added-value chemicals (e.g. functional additives). The production of bio-oil and syngas from lignin is also a growing application that needs further research with regards to process aspects (pyrolysis and gasification). Expanding the use of lignin as feedstock for conversion into materials such as fibres, resins and reinforcement of composites (i.e. thermoplastics, thermosets, bio-based plastics, rubber or foaming materials) is being researched at different TRLs. The strengths of lignin derived materials are the high functionality and the possibility of finetuning their mechanical, optical, and barrier properties due to the inherent lignin structure. The scale up of the developed technologies needs to prove technical and economic feasibility in specific value chains for a more extensive uptake of lignin-based products.

Specific challenges:

- Lignocellulosic biomass feedstock pre-treatment and separation of lignin from other bio-polymers (cellulose and hemicellulose) prior to recovery for further downstream processes;
- Selective lignin depolymerisation and conversion to obtain highly functionalised building blocks, especially focusing on advanced separation and catalysis developments;
- Enhance biomass valorisation via pyrolysis and catalytic pyrolysis through reactor, process and catalyst development to improve on issues related to the properties of bio-oils (e.g. low heating value and high instability at elevated temperatures and pH) and bio-oil upgrading;
- Low temperature catalytic gasification of lignin for syngas production;
- Improve properties for lignin-based composites (driven by the application) such as solubility, access to lignin active sites, organoleptic characteristics (i.e. smell, colour) that might affect the perception of composites and resins upon using unmodified lignin.

Specific expected impact: Lignin-based polymers and promising lignin-based composites can further have impact by enhancing the efficiency and integration of second generation biorefineries. Lignin-derived materials have the potential to be used in buildings and infrastructure, consumer goods, packaging, transport, energy storage and production, health and wellbeing. Lignin can be the source of platform chemicals, and materials. Modified lignin and lignin based functional materials have potential in materials for medical applications. Lignin can provide an abundant alternative feedstock source for aromatic compounds and high value materials, accounting for the 60 to 70 million metric tonnes of lignin available from wood pulp and the paper industry, out of which 95% is currently being burned for energy recovery.

IMPACT EXAMPLES:

Example 1: Up to 85% CO_2 emissions reduction, €400 million turnover in biorefinery intermediates (lignin and sugars) and €650 million in chemical intermediates and products for a 1.5 million ton/year lignocellulose biorefinery are expected by producing chemicals, food and specialties from lignocellulosic feedstock.[37]

Example 2: 90% CO_2 emissions reduction is envisioned by producing lignin-based bio-oil from lignin in black liquor from the pulp industry.[38]

Example 3: Transforming lignin into a biodegradable biopolymer with enhanced properties (e.g. mechanical strength, ultraviolet (UV) light stability and fire-resistance), represents an alternative to plastics such as polystyrene (PS) with an improved environmental profile.[39]

TRL(now) & TRL(2030): The various levels of development of technologies to produce lignin-derived products is highly impacted by feedstock used, the respective process as well as the application. This implies a wide TRL range; albeit the technological readiness for obtaining aromatics (with a high yield and selectivity) remains a challenge. Improving on overall lignin valorisation to a range of products is recommended towards 2030, as part of the development of integrated biorefineries.

2.3.3 Non-lignocellulosic-derived chemicals and polymers

Context: Non-lignocellulosic biomass feedstock is also a source for bio-derived chemicals and polymers. Micro- and macroalgae are growing in importance to provide a wide range of high value products (lipids, proteins, pigments, carbohydrates, vitamins and antioxidants), offering a wide range of applications, including energy, fuels, food, agriculture, cosmetics, textile medical and pharmaceuticals. The development of algae-based fuels is limited by high capital expenditure (CAPEX) and operating expenditure (OPEX) and high-value products could further improve the economics of a microalgae biorefinery. Moreover, the valorisation of chitinous biomass, in particular chitin and chitosan, find applications using either chitosan alone or as a copolymer, nanoparticles and/or nanofibres in the food and water sectors. The antimicrobial properties of chitosan bring advantages in biomedical applications.

Specific challenges:

- Harvesting, dewatering and dissolution technologies to efficiently treat large volumes of biomass;
- Selective separation to obtain homogeneous fractions in relation to molecular size and physicochemical characteristics;
- Application driven properties, such as solubility, low immunogenicity for food, health and medical uses need to be addressed at biomass production levels and/or at the downstream processing steps;

- Scaling up of extraction and downstream processes for micro- and macroalgae;
- High variability of the raw material composition and standardisation challenges for the chitinous biomass-derived products;
- Milder processing conditions for chitin including the use of enzymes and microbes, mechanical depolymerisation and unconventional heating such as microwave and ultrasound.

Specific expected impact:
Non-lignocellulosic biomass valorisation will have an impact on extending the biomass feedstock choices and contribute in expanding the high-value bio-based products portfolio, with applications across existing and new value chains.

IMPACT EXAMPLES:

Example 1: A new algal biorefinery bringing to the market innovative algae-based ingredients for high-end applications, spanning from algal terpenes for fragrances to long-chain terpenoids (carotenoids) for nutraceuticals and cosmetic actives.[40]

Example 2: Converting biomass into valuable products via a homogenisation step with insects to cope with the heterogeneity of side-streams, a new value chain will be elaborated that includes a homogenisation step in the biorefinery approach. Products include proteins and oligopeptides, lipids, chitin, chitosan and derivatives, N-light compost and minor compounds.[41]

TRL(now) & TRL(2030): TRL is impacted by feedstock (e.g. microalgae over chitinous biomass) and final product; targeting TRL > 5 across a wider range of product categories from non-lignocellulosic feedstock is suggested by 2030.

2.3.4 Bio-degradable and / or compostable packaging materials

Context: The European plastics converters demand for plastics in 2018 amounted to 51.2 Mt, out of which 40 % finds its way into packaging applications.[42] Packaging applications require cost effective solutions with suitable performance, while still allowing high recycling rates after use. In multi-layer packaging, each layer is composed of different polymers that perform specific functions, making it difficult to recycle. The end-of-life phase for this packaging, therefore, is either incineration or landfill. Currently, most of food packaging contaminated with food waste ends up being neither reused nor recycled. Packaging materials, once in contact with food waste, are difficult to recycle, with food residues also acting as recycling contaminants.

Food packaging solutions, having removable layers/ coatings, in direct contact with the food so that they can be separated from the main packaging material that has not been in contact with the food, have been under investigation. Biodegradable and/or compostable materials can be used for this layer. Compostable plastics belong to this new generation of packaging materials that are degraded by composting under mild conditions. These materials possess most of the properties of conventional food packaging plastics (such as tensile strength, oxygen barrier properties, resistance to heat, impact or shock), while ensuring degrading in a composting facility under specific conditions.[43] Bio-based materials are not necessarily biodegradable and/or compostable but bio-based polymers, and their often unique functionalities, can be designed and used to produce such materials, such in the case of PLA or other polymers.

***Note:** For waste valorisation processes, applicable to biomass-derived and non-biomass derived plastics waste, please see section* **3.11 (Chapter 3)**.

Specific challenges:
- Control of the thickness of the packaging material layer to achieve degradation efficiency;
- Chemical structure and design to fit the biodegradability/ compostability conditions (e.g. soil);
- Cost competitiveness of bio-based and biodegradable materials;
- New monomers to formulate novel (co)polymers that can be better composted;
- Understanding of chemical routes for the polymer biodegradation (e.g. the presence of unsaturated and amorphous regions susceptible to oxidation);
- Control of the molecular weight of the polymer since with a higher molecular weight, the degradation rate is lower;
- Control of hydrophobicity of the material, as hydrophobicity interferes with the microbial activity and hence hampers the biodegradation;
- Modification of chemical structure: The head-to-head and the tail-to-tail addition of monomer units create weaker portions in the polymer favouring degradation. Likewise, branching increases degradation rate but cross-linking reduces it.

Specific expected impact:
By 2020, the production capacity for bio-based and biodegradable plastics has been projected to account for nearly 2.5 % of fossil-based plastics production, with a growing market.[44] Environmental claims regarding biodegradability or compostability should comply with appropriate European standards and harmonised rules for defining and labelling compostable and biodegradable plastics.[45] Certified compostable food packaging has the potential to increase the valorisation of waste. Compostable packaging products can help to increase organic waste collection and as such contribute to a reduced environmental impact. Regional effects include the reduced need for landfill space, reducing methane emissions from landfill, whereas the production and use of compost could be used for soil improvements in agriculture. However, choices regarding waste treatment need to be made based on assessment not only on product level but on waste stream level.[46]

IMPACT EXAMPLES:

Example 1: Development of recyclable and biodegradable packages for food products, with proper safety characteristics and the production of functional coatings with antioxidant, antimicrobial and oxygen and water/vapour barrier properties. Bio-based, high oxygen/water barrier and active coatings to be used in monolayer bio-based packaging (films and trays) as alternative to current metallised and modified atmosphere packages.[47]

Example 2: Development of processes for an all-cellulose packaging material that can compete with existing multi-layer plastic materials or multi-materials while being both renewable and recyclable in the paper waste value chain and biodegradable.[48]

TRL(now) & TRL(2030): Biodegradable and compostable bio-based materials have reached TRL 4 (polymer and value chain dependent though) and demonstration activities could be explored further for packaging applications by 2030.

2.4 Additives

Context: Additives are often essential to reach desired functionalities and ensure performance (e.g. flame retardancy, UV light and oxidation resistance, among others) as well as durability for materials such as polymers, composites, and coatings. Besides being a key enabler for materials performance, additives have also a direct impact on the recyclability of materials, and consequently on the quality of the recyclates. They can be specifically designed to improve recyclate 'performance', the compatibility of mixed recyclates and to facilitate recycling processes, mainly by increasing effective sorting and separation.

Market, overall expected impact: Additives aim to improve durability and performance of materials, predominately plastics, coatings and resins. A major factor driving the growth of the market is the increasing demand for plastics in emerging economies, given their increasing application in various end-user industries, such as construction, automotive, consumer goods, and packaging.

Additives address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Manufacturing technologies' (4.1), 'Advanced materials' 4.4, 'Circular Industries' 4.8, 'Communities and cities' (5.5), 'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), and 'Circular systems' (6.7) mainly by the following factors:

- **Safety of recycled materials** by using additives that do not negatively affect the properties of the recyclate when it is used to produce a new product;
- **Tracking to improve recycling** and **sustainability** by the adoption of controlled labelling, tracing, sorting and separation technologies for an optimised industrial recycling process;
- **Durability of materials through novel types of additives** allowing enhanced mechanical and/or physicochemical properties.

Horizontal challenges:

- Circular and safe-by-design approaches for the development of novel additives with target performance for improved durability;
- Application of eco-design principles and recyclability strategies to improve recovery and recyclability rates of materials/polymers by choice and design of additives.

SUSCHEM PILLARS – MULTI-KETS:

Related innovation under **Advanced Processes (Chapter 3)** includes: 'Enabling waste valorisation via catalysis' (3.9.2), 'Separation process technologies' (3.3), and 'Chemical recycling of plastics waste' (3.11.1).

Enabling Digital Technologies (Chapter 4) will have an expected contribution on additives-related innovation via: 'Materials and molecules design: modelling and simulation developments' (4.1.1), 'Materials and formulations design–integration with process design' (4.1.2), 'Industrial data platforms' (4.7.1), and 'Enabling transparent supply chains' (4.9.1).

Within **Advanced Materials** the relevant topics include: 'Composites and cellular materials' (2.1), '3D- printable materials' (2.2), 'Biocompatible and smart materials' (2.5), 'Materials for electronics' (2.6) and 'Coating materials and aerogels' (2.9).

RD&I Actions

2.4.1 Additives for tracking, sorting and separation

Context: The composition and homogeneity of waste streams can be variable, depending on the source and nature of the waste. Some plastic waste streams comprise mainly one polymer type, such as collected PET bottle streams. On the contrary, other plastic waste streams can be complex mixtures of different polymers, multi-colour, multi-layer or multi-material articles, and these present a bigger challenge in terms of sorting and separation. The use of a range of tracing additives is expanding in this application due to their adaptability to the matrix materials, their controlled safety-by-design and the small amounts needed.

Specific challenges:

- Development of additives for tracer-based sorting such as UV-tracing able to detect specific light signals emitted (or absorbed) by the polymers and/or additives. Tracing additives must be adaptable to different material matrixes bearing different physicochemical properties, for improved detection and sorting;
- Complement additives innovation with improvement in identification techniques used for material sorting (e.g. improvement of optical sensors for better spatial recognition along with the use of additives would allow to automate sorting to higher speed, accuracy and lower detection limits).

Specific expected impact: There is an urgent need for efficient materials sorting and separation in high-volume applications such as packaging, textiles, automotive and transport, agriculture, consumer goods, health, construction and industry. Increasing consumer awareness and policies in line with the EU Strategy for Plastics in a Circular Economy will allow recycling rates to grow even higher, to the target of more than half of plastics waste generated in Europe being recycled by 2030.

IMPACT EXAMPLES:

Example 1: Near infrared (NIR) reflective reflective and transparent alternatives to carbon black for colouring plastics. The colourants enable the current NIR sorting operations to segregate black and coloured plastics from streams, to a purity suitable for high-value recycled engineering polymers.[49]

Example 2: Smart sorting technologies to separate a diverse range of polyurethane (PU) materials into dedicated feedstock for chemical recycling into new products, with a target 90 % recovery of end-of-life PU.[50]

TRL(now) & TRL(2030): Current TRL starts at 5, although for some particular novel technologies (e.g. identification of organic legacy additives) the TRL is 2, and further innovation and demo actions are suggested.

2.4.2 Additives and compatibilisers for complex compositions

Context: Composites, multi-phase or multi-layered structures, as well as coated materials cover the increasingly demanding requirements of many applications. However, there has been a rising concern on the end-of-life possibilities for these materials, and an urge to find efficient and cost-effective recycling, without impairing functionality during their lifespan. Additives as compatibilisers may bring beneficial features from the point of view of recyclability.

Specific challenges:

- Compatibilisers for the growing range of potential mixtures of polymers from multi-component products;
- Specific (reversible) adhesives or additives to facilitate recyclability of multilayer materials into high-purity streams of individual layer components;
- High-efficiency and functionalities in the final product, while not impairing recyclability.

Specific expected impact: Improved compatibilisers and additives will impact on the recycling yield as well as enhance the homogeneity of the waste streams, allowing for high-quality recycled products; hence overall contributing to a more circular economy.

IMPACT EXAMPLES:

Example 1: Solvent-free recycling process for post-industrial vulcanised Ethylene propylene diene monomer (EPDM) rubber scrap material with the use of liquid EPDM polymers as additives into high-quality secondary products, enabling the substitution of up to 80 % of virgin EPDM rubber.[51]

Example 2: Novel triggerable material systems based on smart additives (like microcapsules or microwave triggered additives) for 'coating' applications that will be activated by a specific trigger, enabling coating removal and easy recycling of coated parts.[52]

TRL(now) & TRL(2030): TRL is in the range of TRL 2-4 for technologies based on the use of reversible additives and advanced nano-additives, while TRLs of 5-6 refer to the next generation of compatibilisers for multicomponent products and the recyclability of thermosets. TRLs expected to be achieved by 2030 are 5-8, by the development mostly of specific innovation actions.

2.5 Biocompatible and Smart Materials

Context: Biocompatible materials are meant to interact with biological systems but also find applications as drug carriers and delivery systems. Their applications span from grafts such as heart valves, to artificial joints and personalised medicine. Features required from biocompatible materials are non-toxicity, along with characteristic properties (mechanical, biological and/or chemical) according to the required application (internal or external use in the body, permanent or limited to a specific life span). Smart drug delivery systems constitute an application of increasing demand since they enable minimisation of the side effects of the applied drug as it is targeted specifically to the area of the body/organ to be treated. This is achieved by tuning the carrier's material chemistry to achieve targeted release of an active compound upon a certain trigger. The formulations and physical form of these smart carrier materials are also adapted to the specific needs of the application route (e.g. oral, pulmonary, injectable, implantable, transmucosal).

Market, overall expected impact: Biocompatible and smart materials offer advanced functionalities in biomedical solutions. The global market for biocompatible materials and pharmaceutical drug delivery is expected to be further driven by the rising prevalence of chronic diseases, the growth in the biologics market, technological advancements and new product launches.

Biocompatible and smart materials address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Health throughout the life course' (1.1), 'Tools, technologies, and Digital solutions for Health & care, including personalised medicine' (1.5), 'Manufacturing technologies' (4.1), 'Emerging technologies' 4.3, 'Advanced Materials' 4.4, and 'Bio-based innovation systems in the EU Bioeconomy' (6.6), mainly by:

- **Biocompatible materials** for medical devices and implants positively contribute to the short- and long-term health of citizens and to expand personalised medicine;
- **Smart drug delivery systems** improve the efficiency of pharmaceuticals by decreasing the doses of drugs while minimising side effects.

Horizontal challenges:

- Developing biocompatible materials for tailored and long-life use in medical applications;
- Materials that can prevent biofilm formation to be used in long-term devices (bacteria-resistant medical devices);
- Smart drug delivery materials adapted to the most difficult delivery routes (e.g. pulmonary, brain barrier);
- Improved characterisation of biocompatible materials with advanced analytical techniques to understand the relationship between the desired morphology and chemical structure.

SUSCHEM PILLARS – MULTI-KETS:

Enabling Digital Technologies (Chapter 4) will accelerate and facilitate the design and production of safe biocompatible and stimuli-responsive materials mainly via: 'Materials and molecules design: modelling and simulation developments' (4.1.1), and 'Materials and formulations design– integration with process design' (4.1.2).

Contributions of innovation in **Advanced Processes (Chapter 3)** for the synthesis on novel therapeutics, or relevance to stimuli-responsive biocompatible materials include: 'New reactor design concepts and equipment' (3.1) and 'Industrial Biotechnology' 3.10.

Within **Advanced Materials** the relevant topics include: 'Composites and cellular materials' (2.1) and '3D-printable materials' (2.2).

RD&I Actions

2.5.1 Biocompatible stimuli-responsive drug delivery systems

Context: Biocompatible stimuli-responsive materials have the potential to deliver pharmaceuticals or biomolecules to a specific cell or region within the body to induce local action. The response is triggered by physical and chemical stimuli (e.g. pH, redox potential, temperature, ionic strength or the presence of enzymes) that produce specific changes to the material for it to release an active component. Formulations that result in sustained active drug levels in the body will directly result in improved treatment efficacy. Several stimuli-responsive materials are currently used or in development for these purposes, such as: a) electro-responsive polymers, capable of changing dimensions and/or shape in response to electrical stimuli. Examples of these materials, suitable for drug delivery, are hydrogels such as chitosan or hyaluronic acid, due to their biocompatibility, degradability and hydrophilicity;[53] b) magneto-responsive polymers, consisting of inorganic magnetic nanoparticles physically entrapped or covalently immobilised in a three-dimensional cross-linked network, finding application for delivery of drugs under magnetic fields, c) thermo-responsive polymers, but also d) photo-responsive polymers with applications in tissue engineering, reversible optical storage as well as drug delivery. Other biocompatible stimuli-responsive materials include metal organic frameworks composites-based options, materials with reversible sol-gel transitions near body temperature and ultrasound responsive polymers.

Key specific challenges:

- Improvements in electro-responsive polymers which require less conductive media for activation;
- Alternative isomerisation for photo-responsive polymers since UV irradiation is a limitation for biomedical applications;
- Longer term stability of Metal Organic Framework (MOF) composites in physiological media;
- Enhancing the biocompatibility of polymers for thermo-responsive applications;
- New potential formulations for ultrasound responsive polymers and nanocarriers are required.

Specific expected impact:
Stimuli-responsive, bio-inspired smart materials and smart drug delivery systems hold great promise in biomedical and industrial applications. Applications and impact could expand from on-demand drug delivery and actuators to tissue generation/repair, biosensing, smart coatings, and artificial tissues.

IMPACT EXAMPLES:

Example 1: Development of a dual stimuli-responsive hybrid polymer/iron oxide nanocubes (IONCs) delivery system to combine magnetic hyperthermia (MHT) with myeloid-derived suppressor cells (MDSC) depletion-targeted immunotherapy for intra-tumoral treatment of Glioblastoma (GBM), characterised by its extremely poor prognosis.[54]

Example 2: Development and validation of stimuli-responsive nanocapsules able to encapsulate efficiently and protect specific active ingredients for skin care application.[55]

TRL(now) & TRL(2030): Stimuli-responsive materials with highly demanding functionalities for biomedical applications are currently at TRL 3 for many applications. Research would be needed on disruptive concepts using biocompatible stimuli-responsive materials for biomedical applications. More innovation and demonstration actions will be needed for existing stimuli-responsive materials to prove feasibility regarding risk minimisation, performance and long-term biocompatibility.

2.6 Materials for Electronics

Context: Most printed, flexible and organic electronics consist Organic Light Emitting Diodes (OLEDs); printed biosensors and printed conductive ink (predominately for photovoltaics). Additional applications for materials for electronics, such as stretchable and wearable electronics, flexible batteries, capacitive sensors and healthcare devices have strong growth potential. Increasing research & development activities are ongoing in the field of materials for electronics and are building on the base for a new generation of higher performance electronics. The sector is advancing at rapid pace with technologies readily available for commercial use and emerging technologies with disruptive impact anticipated to be available within the next 3-5 years.[56] Furthermore, the advances in the developments of electronic materials enable a more sustainable production of electronic devices. Key and upcoming research areas include sensor technologies, thin film and multi-junction photovoltaics as well as materials for quantum computing.

Market, overall expected impact: Materials for electronics and sensors have a vast array of applications in industrial automation, transport, aviation, mobile devices, consumer items, building and infrastructure, medical equipment, security applications, IT infrastructure and communications. The market for printed, flexible and organic electronics will grow from $31.7 Billion in 2018 to $77.3 billion by 2030.[57] The stretchable electronics market is foreseen to grow at 80% CAGR (2018-2023).[58]

Materials for electronics address several Horizon Europe (HEU) clusters and areas of intervention: 'Tools, technologies, and digital solutions for health and care, including personalised medicine' (1.5), 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced materials' 4.4, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Communities and cities' (5.5), 'Industrial competitiveness in transport' (5.6), 'Smart mobility' (5.8), and 'Circular systems' (6.7) by:

- **Enabling the production of a wide range of new electronic devices with applications in healthcare, consumer electronics, energy, buildings and mobility**;
- **Facilitating sustainable manufacturing of novel electronics including sensors, displays, photovoltaics** through easier to process materials (e.g. printable, water soluble), resulting in the reduction of waste during the manufacturing process of such products.

Horizontal challenges:

- Integration and scale-up of novel materials into the existing production/manufacturing environment;
- Complexity of testing and qualifying the performance of the new materials in the final applications;
- Longevity, reliability and robustness of the final product needs to be ensured when the novel materials are introduced;
- High purity requirements for materials implying stringent purification technologies.

SUSCHEM PILLARS – MULTI-KETS:

Enabling Digital Technologies (Chapter 4) will accelerate and facilitate the design and production of materials for electronics, including sensors: 'Laboratory 4.0-Digital R&D' (4.1) and 'Process analytical technologies (PAT)' 4.2

Within **Advanced Materials** the relevant topics include: '3D-printable materials' (2.2) and 'Materials for energy storage' (2.8).

RD&I Actions

2.6.1 Sensors dedicated materials

Context: Sensors that are printed on flexible substrates represent a growing market, the biggest segment today is blood glucose test strips. The next generation

of printed sensors (biosensors, capacitive sensors, piezoresistive sensors, piezoelectric sensors, optical sensors, temperature sensors, humidity sensors, gas sensors) will enable applications, including human-machine interfaces, environmental sensing, sensors for packaging, and battery embedded sensing. These sensors benefit from materials innovation and technologies developed by the chemical sector. While some may consist of a very simple structure with only a few electrodes, others are much more complex and require the deposition of multiple layers. What they have in common is the capability to be manufactured on plastic substrates, which offer advantages in terms of mechanical flexibility, thinness and weight reduction. In this respect compatible inks for printed electronics as well as new polymeric substrates compatible with the inks are still in an early stage.

Key specific challenges:

- Developing substrates and materials for layering;
- Development of material inks suitable for sensors printing (e.g. non -impact printing);
- Development of materials for fluorescence-based sensors and electrochemical biosensors.

Specific expected impact: Sensors will create new business opportunities. Sensor systems and electronic instrumentation are the highest growing and upcoming segments in the semiconductor market. The introduction of new electronic materials for sensors such as printable conductors and semiconductors is likely to lower the cost, weight and size of electronic devices and will help spur demand for a growing sensor market.

IMPACT EXAMPLES:

Example 1: Polymer-based printed electronics, suitable for next generation portable, wearable short-range wireless communicating devices with low power consumption. High-frequency printed and direct-written organic-hybrid integrated circuits were fabricated with scalable processes at low temperature on a plastics substrate.[59]

Example 2: Flexible and stretchable photonic ribbons and fibres, prepared by directing the flow of optical materials through innovative solid-state dewetting and thermal drawing processes.[60]

TRL(now) & TRL(2030): Many technologies are available at TRL 3-5. Further research and innovation actions in the field of advanced materials for sensors will allow TRL levels to be 6/7 by 2030.

2.6.2 Thin film and organic photovoltaics

Context: Using less silicon without hampering the performance is the drive for the next generation of photovoltaic (PV) cells. The cells need to be more efficient and economically sound, suitable for mass manufacture and able to operate for decades with a minimal environmental footprint. Developments in thin film photovoltaics have been progressing fast over the past few years. For example, CdTe, CuInGaSe2, and perovskite thin film solar cells have all demonstrated greater than 20 % conversion efficiencies. This is mainly due to the progress in understanding and developing new materials and device structures and improvement in processing steps. Moreover, organic photovoltaic (OPV) materials also offer a promising form of PV cells, relying on organic substrates such as polymers. These offer the advantage of good performance under indoor lighting conditions, low capital expenditure, cell flexibility and potentially simplified manufacturing processes by using printing technologies on plastic substrates. Due to their lightweight, flexible and semi-transparent properties, OPV cells could be used in building integrated photovoltaics (BIPV) incorporated into building facades. OPV market is segmented into polymer, small molecule and perovskite-based cells. Very recent technologies are also exploring luminescent solar concentrators (LSC) that gather light and funnel it into a smaller highly efficient solar cells.

Key specific challenges:

- Novel materials to allow lower cost and low-temperature processes to manufacture perovskite cells;
- Alternative high purity molecules and polymers suitable for organic photovoltaics with low batch-to-batch variation;
- Materials enabling luminescent solar concentrators;
- Developing coating materials to enable self-cleaning, anti-soiling and anti-reflective properties.

Specific expected impact: The global thin film PV market is expected to grow and will readily benefit from solutions with enhanced efficiency. Exploiting new markets that can become transformative in the long term, such as the building integrated photovoltaics, is envisaged.

IMPACT EXAMPLES:

Example 1: Solid-state lead halide perovskites, used as thin-film photovoltaic device class, leads to a high power conversion efficiencies (22%) and stabilities (> 1000 hours at 80˚C under 1 sun illumination). The production of the final perovskite thin-film can be achieved with low-temperature fast processes. This makes halide perovskites cost efficient, and promises to deliver a PV technology with a levelled cost of electricity (LCOE) below existing mainstream PV.[61]

TRL(now) & TRL(2030): Technologies in this area have varying TRL levels. New developments such as organic PV cells and LSCs are still in early phases of research (TRL 1-2), whereas other technologies such as BIPV thin film are further advanced (TRL 4-5) but need to overcome market barriers before a wider uptake is achieved.

2.6.3 Multi-junction photovoltaic materials

Context: One approach to overcome existing PV cells efficiency limitations is to form multi-junction cells. The top cell absorbs one part of the light spectrum and the unused light passes through it before being absorbed by the lower cell. Tandem cells and triple cells are commercially available but with scope for improvement. A recent class of materials, perovskites, is being developed in thin film cells. These cells can be produced by cheap, low temperature solution processing and the structure of the perovskite compounds is relatively easy to fine tune, thus enabling modifications of their optical and electronic properties. To improve the performance of all thin film multijunction devices, the cells will need better interfaces between the materials. Research is evolving also to tandem crystalline silicone/perovskite or Replace with 'crystalline silicon/ Copper zinc tin sulfide (CZTS) and on the integration of semiconductors with silicon-based microelectronics.

Key specific challenges:

- Complexity of the use of several different materials stacked in multiple layers;
- Wide band gap chalcogenide and/or perovskite-based absorbers minimising or eliminating use of critical raw materials.

Specific expected impact: The high performance and efficiency, capture of energy in larger ranges of wavelength of the incident light, due to the different band gaps, will allow to expand the use of PV in more efficiently demanding applications and sectors.

IMPACT EXAMPLES:

Example 1: Power conversion efficiency of perovskite/silicon tandem cells and currently at > 27%, significantly exceeding that of silicon only PV cells.[62]

TRL(now) & TRL(2030): Materials for multijunction PV cells are still at research levels (TRL 3-5). More innovation actions on exploring novel materials for the development of multijunction PV cells would need to be considered by 2030, allowing for demo actions towards cost efficient and environmentally friendly production processes.

2.6.4 Materials for quantum computing

Context: Quantum computing takes advantage of the ability of subatomic particles to exist in more than one state at any time. Due to the way such materials behave, computing operations can be done much more quickly and use less energy than with classical computers. In this context the field of enabling quantum materials has seen an exponential rise in research interest over the past two decades. Graphene is also considered as a promising candidate material for quantum computing.

Key specific challenges:

- Developing materials with strong electronic correlations, superconducting, magnetic order and materials whose electronic properties are linked to quantum effects.

Specific expected impact: Quantum materials will enable the next generation of ultrafast supercomputers. Quantum computers will largely contribute to new discoveries in the areas of healthcare, energy, environmental systems, and smart materials, amongst others.

IMPACT EXAMPLES:

Example 1: Chemical processing and functional applications of graphene and graphene-related materials for engineering new molecular structures suitable for quantum computing.[63]

TRL(now) & TRL(2030): Materials for quantum computing are at low TRL. It is expected that due to the supercomputer capacities demand that is to be addressed by quantum computing, research activities to raise these materials' TRLs by 2030 will need to be undertaken.

2.7 Membranes

Context: Membrane technologies have become versatile separation tools. In several industries membrane processes have successfully replaced classical separation technologies (e.g. distillation, extraction, precipitation) due to energy efficiency and selectivity. Membranes are established already for water desalination or water purification but also in the production of food and beverages and biotechnology-based processes. Within the chemical sector, separation technologies account for 50-90 % of operational expenses within a production process.[64] Membranes often have lower energy demands for separations and therefore are very cost efficient in comparison to other available techniques (e.g. they use 90 % less energy than distillation processes).[65] Beyond water treatment, membranes are used in separations applicable for mixtures of gases as well as organic and/or inorganic substance separations. In all cases, membrane material optimisations are required to further improve the performance of established technologies but also to access additional application areas. Improvements are needed in the selectivity of existing membranes by better pore size control, boosting their lifetime by increasing chemical resistance in demanding media (oil & gas production, chemical production, biotechnology). Development of membrane technologies without reduced requirements for solvents, modification tools to address the fouling propensity of membranes as well as the combination of separation tasks within a single membrane need to be addressed.

Market, overall expected impact: Membranes contribute to energy and overall efficiency of chemical and biotech processes (see 'Separation process technologies' under Chapter 3: Advanced Processes **(3.3)**).

Advanced materials for membranes address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Health throughout the life course' (1.1), 'Manufacturing technologies' (4.1), 'Advanced materials' 4.4, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Energy supply' 5.2,'Buildings and industrial facilities in energy transition' (5.4), 'Communities and cities' (5.5), 'Agriculture, Forestry and rural areas' (6.3), 'Food systems' (6.5), and 'Circular systems' (6.7) by:

- **Improved efficiency in gases production and/or gas mixtures separation/purification prior to valorisation to chemicals and fuels** (e.g. H2, CO_2)[66 67];
- **Improved resource and energy efficiency in chemicals production**, including platform chemicals, fine chemicals, or polymers by improving selectivity and purification efficiency (upstream and downstream) and recovering reaction substrates, catalysts, and solvents at potentially lower energy input and reducing resource and energy requirements;
- **Recovery of valuable materials** such as metals or critical raw materials (CRMs) from concentrated waste (e.g. Waste electrical and electronic equipment (WEEE)), industrial streams or water sources (e.g. wastewater, saline water and brine) will allow for circularity;
- **Water treatment and seawater desalination** at lower energy requirements.

Horizontal challenges:

- Developing new materials for enhancing the membranes' selectivity and performance;
- Reduction of the energy required for membranes production.

SUSCHEM PILLARS – MULTI-KETS:

There is strong relevance between innovation in advanced materials for membranes and **Advanced Processes (Chapter 3)**: 'Membrane reactors - integrated systems' (3.1.6), 'Membranes integration in continuous processes' (3.3.1), 'Hydrogen production with low-carbon footprint (3.7)', 'Catalysis' (3.9), 'Industrial biotechnology' 3.10, 'Waste valorisation process technologies' 3.11 and 'Process technologies for advanced water management' 3.12.

Enabling Digital Technologies (Chapter 4) will accelerate and facilitate the design and production of 'Materials and molecules design: modelling and simulation developments' (4.1.1) and 'Materials and formulations design–integration with process design' (4.1.2).

There is a horizontal impact with regards to the production of **Advanced Materials** and especially 'Bio-based chemicals and materials' (2.3).

RD&I Actions

2.7.1 Membranes for separations in diluted conditions and water treatment applications

Context: Membranes play a relevant role in conditioning process water and wastewater treatment. Membrane modules are used for high-quality water or they

are applied in combination with bio-processes in wastewater treatment (membrane slurry reactor). In the context of water loop closure, membranes can enhance water reuse rates while also increasingly dealing with concentrate/residue treatment. To-date, polymeric membranes make up most membranes used in applications, including water purification to provide drinking water, resource recovery for critical raw materials recycling as well as the removal of micro-pollutants from wastewater. Recently ceramic and hybrid ceramic - organic membranes have emerged as an alternative in water treatment. The main benefit of these membranes is that they have a high chemical and thermal stability that allow cleaning or regeneration by use of steam or chemicals.

Specific challenges:

- Fouling of membranes for water applications;
- Membrane selectivity for removal of specific impurities from highly concentrated residue streams and valorisation of these streams;
- Energy efficiency of membranes for water treatment under high salinity and organic loading;
- Installation of membrane modules and reduction of CAPEX and OPEX.

Specific expected impact:

Membranes have a significant impact on sustainable treatment of water, ranging from surface and ground water to wastewater and desalination to produce drinking water. Additionally, with increasing pressure being placed on natural resources, the efficient use and recovery of resources from wastewater is becoming of greater importance to society. Further impact of membranes is envisaged in saving freshwater resources by increasing the water efficiency and water reuse rates in industry. Overall, membranes positively affect the environmental value of water efficiency measures in industry and bring significant contribution to the circular economy of the concentrate/residue streams through wastewater treatment.

IMPACT EXAMPLES:

Example 1: Sustainable water treatment by multi-functional and low-cost polymeric membranes for water treatment and desalination. The main innovation resides in the combination of enhanced structural properties (high porosity and reinforcement) for improved desalination and light-induced antifouling and antimicrobial activity based on the loading of photosensitisers in the polymeric membrane.[68]

TRL(now) & TRL(2030): For some applications in water treatment (e.g. concentrate treatment for disposal, close-to-loop closure treatment) technologies are currently at TRL 5. Anti-fouling membranes based on modified ceramic membranes and hybrid organic - inorganic membranes are currently at TRL 4-6, whereas membranes to recover resources from water (metals) are at TRL 1-3.

Demonstration activities to achieve scale-up by 2030 would be needed for the anti-fouling aspects of membranes. For concentrated streams treatment, demonstration activities need to be undertaken to achieve TRL 6-8 by 2030. Research to reach a TRL 4-5 by 2030 needs to be considered for membranes for resource recovery applications.

2.7.2 Membranes for gas separations - membrane distillation

Context: Membrane distillation combines some unique characteristics of both membrane and distillation processes. It is modular and space-saving, operates at mild temperatures (50 – 90°C) and pressures (atmospheric pressure or vacuum). Different from other pressure-driven membrane processes, its separation performance is less affected by the feed concentration and its energy source can be solar energy or waste heat instead of electricity. Membrane distillation is one of the key process elements used for the removal of gas/volatile pollutants in wastewater from industrial chemical plants as well as for resource recovery (ammonia, alcohols) for recycling. Traditionally, microporous polypropylene (PP), polyvinylidene difluoride (PVDF) and polytetrafluoroethylene (PTFE) membranes are employed as membrane distillation membranes with good short-term performance as they combine low resistance to mass transfer with low thermal conductivity to prevent heat losses across the membrane. Future membrane distillation membranes must have the characteristics of omniphobicity so that they are able to repel both high and low surface tension compounds.

Specific challenges:

- Long-term performance challenges: Scaling, wetting and complexity of feeds;
- Chemical inertia of typical hydrophobic materials, limiting the effective manipulation of surface morphology;
- Need to simplify the design of omniphobic membranes (e.g. by using 3D-printing technology);
- Use of safer solvents during the fabrication of membranes to minimise environmental impact;
- Combination of membrane distillation with solar heating or photo-thermal elements to minimise energy consumption.

Specific expected impact: Membrane distillation for energy efficient separation of gases will achieve a significant impact on reducing CAPEX as it allows using smaller size equipment as well as operating at lower temperatures than standard distillation and with the additional advantageous possibility to use low grade heat or renewable energy.

IMPACT EXAMPLES:

Example 1: Porous metal organic framework (MOF) able to separate CO_2 from a gas stream (including methane, nitrogen, oxygen, hydrogen, olefins, etc.) exhibiting CO_2/CH_4 selectivities at least one order of magnitude higher when compared with current state-of-the-art models.[69]

Example 2: Recovery of gaseous ammonia from animal barns to produce nitrogen fertiliser through the development of a gas-permeable membrane, achieving a 60-80% reduction in the concentration of ammonia in liquid manure.[70]

TRL(now) & TRL(2030): Membrane distillation for separation of gases is currently at TRL 4-6. Demonstration activities need to be developed to move towards scaled-up applications by 2030.

2.7.3 Membranes for organic and/or inorganic separations (concentrated systems)

Context: The range of available membranes, stable across a range of organic solvents, is somewhat limited. Polymeric membranes tend to be only stable in specific types of solvents with the polar aprotic solvents presenting the greatest issues. In contrast, ceramic membranes, i.e. those based on metal oxides such as TiO2, ZrO2, Al2O3 etc., have far greater stability range in organic solutions than the polymeric equivalents but, due to the highly polar nature of their surface, efficiency is lost in more polar solvents. The range of solvents suitable for use with ceramic membranes can be enlarged by addition of an organic top layer on the surface of the membrane. These hybrid membranes have demonstrated complementary properties to their non-hybrid counterparts and maintain high flux even under high pressure. They find applications in several industrial processes such as lignocellulose separations, low energy solvent separations (e.g. non-thermal solvent exchange), fatty acids isolation and purification, recovery or recycling of bio- and chemical catalysts, and sustainable synthesis through membrane integrated processes or solvent recycling. Hybrid inorganic-organic membranes are highly promising, but further R&D is required to reach their full potential.

Specific challenges:

- Broadening the range of solvent compatibility of the membranes;
- Developing suitable membranes for isomer separations, chiral separations, separations of molecules of similar molecular mass;
- Improving the resistance to fouling effects;
- Understanding the underlying separations mechanisms.

Specific expected impact:
Membranes for organic and inorganic compounds separations will allow to achieve significant impact on reducing energy requirements and CO_2 emissions. Further, they will open new routes to valorise alternative carbon feedstock from sustainable sources such as lignin or fats and oils.

IMPACT EXAMPLES:

Example 1: Ultrathin organic solvent nanofiltration (OSN) membrane, comprising MOF nanosheets in ultrathin polymer matrix in the form of mixed matrix membranes (MMMs), achieving organic liquid separation on a molecular scale with less than half the energy consumption of conventional distillation processes.[71]

Example 2: Membrane separation techniques working at room temperatures and able to achieve separations at the molecular level, i.e. pervaporation and OSN.[72]

TRL(now) & TRL(2030): Ceramic membranes, modified by phosphonic acid derivatives or direct metal - carbon bonded substitution, are currently at TRL 6-7. Hybrid organic-inorganic membranes based on polymeric membranes are at TRL 3- 5. For some applications modified ceramic, polymeric and hybrid organic-inorganic membranes are expected to reach TRL 9 by 2030. For more challenging separations such as those used in the lignocellulose depolymerisation processes, oil component purification or isomer/chiral separations the TRL will be expected to reach 6-7 by 2030 by further RD&I.

2.8 Materials for Energy Storage

Context: Batteries serve a wide range of applications, from transport to consumer electronics and a variety of technologies are available to satisfy the different requirements. The blooming of e-mobility solutions, such as electric vehicles as well as the constantly growing power demands in consumer electronics, drive the development of sustainable and affordable systems with higher energy and/or power density, extended lifetime and wider temperature operation range. Preferably all these parameters should be fulfilled simultaneously while meeting high safety standards. Moreover, as renewable energy becomes increasingly available and less expensive, Europe is looking to make the intermittent renewable energy sources easier to store. One of the energy storage options are batteries for both mobile and industrial stationary applications.

Overall, accelerated research and innovation will be needed to support advanced and disruptive technologies but also the transition to a circular economy for batteries, towards 2030.[73]

Market, overall expected impact: By 2030, there will be a real shift to low- and zero-emission vehicles, including electric cars, while 70 % of European electricity should be produced by renewables and batteries will have a vital role in this transition to clean mobility and energy systems, as foreseen in the EU Action Plan on Batteries.[74] For instance, global electric vehicles sales have been evolving rapidly, from 36 000 units sold in 2011 to more than 1.2 million in 2017 and that number could almost quadruple by 2020.[75] Despite this being the market with the largest foreseen growth for rechargeable batteries, electronic devices still account for 50 % of the sales of lithium-ion batteries.[76] Overall, the next generation of smart, sustainable and durable batteries will exploit the potential of new materials, chemistries, smart functionalities and novel cell designs but also improvements in recyclability.

Materials for energy storage address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Manufacturing Technologies' (4.1), 'Advanced Materials' 4.4, 'Advanced Computing and Big Data' 4.7, 'Circular industries' 4.8, 'Space including earth observations' (4.10), 'Energy supply' 5.2, 'Buildings and industrial facilities in energy transition' (5.4), 'Communities and cites' (5.5), 'Industrial competitiveness in transport' (5.6), 'Clean, safe and accessible transport and mobility' (5.7), 'Energy Storage' (5.9) and 'Circular systems' (6.7), mainly by the following factors:

- **Increased battery reliability with batteries incorporating smart functionalities**, including sensors to monitor parameter changes (e.g. chemical composition, strain, temperature and pressure within the cell) or embedding smart functionalities into the battery cell by integrating sensing technologies (optical, electric, thermal, acoustic or electrochemical) to transmit information in/out of the cells;[77]
- **Increased battery durability**, for example by introducing **auto-reparable or self-healing materials**. This can include supramolecular architectures physically or chemically cross-linked, separators capable of accommodating specific molecules/polymers and release them on demand by physical and chemical stimuli to repair the electrode / electrolyte interface;
- **Improved recyclability**, by developing battery recycling technologies and the implementation of circular economy approaches in **battery design and manufacturing**. Additionally, such strategy shall account for the recovery of critical raw materials (CRMs) from batteries to secure the supply of strategic raw materials for EU industries;[78]
- **Improved cost efficiency and flexibility of next generation batteries** for the implementation of batteries in a wider number of applications, implying small scale, flexible, safe and clean battery solutions;
- **Improved energy storage with applications** in renewable energy sources by exploiting the possibilities of advanced materials.

Horizontal challenges:

- Development of materials allowing improved energy and power density at lower cost. Material performance improvements, i.e. involving higher active surface materials;
- Improved manufacturability by integration of compact, safe, durable and reliable battery materials, complementing battery system development with advanced manufacturing and assembly technologies;
- Enhanced recyclability of materials in line with the concepts of the Circular Economy Strategy.

SUSCHEM PILLARS – MULTI-KETS:

Innovation in advanced materials for energy storage brings links with priorities under **Advanced Processes (Chapter 3),** especially 'Critical raw materials recovery from waste' (3.11.3), and 'Power-to-chemicals' .

Relevant innovation priorities under **Enabling Digital Technologies (Chapter 4)** include: 'Materials and molecules design: modelling and simulation developments' (4.1.1), 'Materials and formulations design– integration with process design' (4.1.2), and 'Distributed ledger technologies' 4.9.

Within **Advanced Materials**, the relevant topics include: 'Composites and cellular materials' (2.1), 'Materials for electronics' (2.6) and 'Membranes' (2.7).

RD&I Actions

2.8.1 Materials for lithium-ion batteries.

Context: Lithium-ion batteries (LIBs) have become a standard in consumer electronics (smartphones, laptops, etc.), but are also used in transport, electric vehicles (EVs, HEVs, PHEVs) and in space applications, as they are amongst the most powerful of the rechargeable batteries on the market today. However, they still need to ensure their long-term sustainability by developing new methodologies and technologies to allow dismantling and recycling, and face some remaining challenges which include improvements in performance.
Li-ion batteries are mature and robust systems, with adequate energy and power density for a multitude of applications. Cathode composition is the main differentiating factor between Li-ion technologies. Currently, there are several LIB technologies. All types of LIBs use lithium ions as the charge carriers between the anode and the cathode, with the majority having graphite as the anode. These anode chemistry archetypes are the basis for specific cathode "recipes". Introducing alternative materials such as lithium manganese nickel oxide (LMNO) or graphite-based and silicon-based electrodes is being explored.

Specific challenges:

- Reducing cobalt content in the cathode while increasing the nickel content to improve performance;
- Increase gravimetric and volumetric energy and power density of battery cells for mobility applications;
- Increase of volumetric energy density for stationary batteries;
- Increase lifetime and temperature operating range of batteries;
- Designing materials suitable for reusing battery components (electrodes, electrolytes, separator membranes);
- Decrease charging time.

Specific expected impact: Contributions to clean mobility and energy systems as well as circularity provided circular design considerations. (please see **Market, overall expected impact (2.8)**).

IMPACT EXAMPLES:

Example 1: Use of graphene-related materials and other two-dimensional crystals and scaffolds to develop batteries (Li-ion, Li-air, Li-S and Na-ion), supercapacitors and devices for hydrogen storage.[79]

Example 2: Lithium-ion based energy storage system offering in-service time of 20 to 25 years, using latest generation of anode materials based on silicon.[80]

TRL(now) & TRL(2030): Current TRL levels are in the range of 5-7 for further advances for materials for lithium-ion batteries. Further Innovation actions will allow a wider European deployment and market implementation by 2030.

2.8.2 Redox flow batteries

Context: Redox flow batteries find applications in energy storage in the grid (i.e. from solar and wind capacities). Flow batteries differ from other storage devices as the energy is stored in the electrolyte. This implies that the energy storing compounds may be charged or discharged in separate units from the cell itself. This offers significant advantages in terms of scalability. Technologies, currently under development, range from redox flow (reduction-oxidation) to hybrid flow (one or more electroactive components are stored as a solid layer) and others. Most advanced flow batteries rely on vanadium chemistry. Given the current low energy densities, flow batteries allow only for stationary applications. A decrease of manufacturing costs and increase of lifetime should be the focus of R&I activities to expand their implementation.

Specific challenges:

- Development of high-efficiency electrodes with enhanced wetting behaviour to the electrolyte;
- Reduction of self-discharge effects that reduce capacity and operating life;
- Scaling of capacity to cover longer ranges from kWh to GWh;
- Increase volumetric density of stationary batteries;
- Improved cell components and pack design for recyclability;
- Integration of system control devices (sensors, power electronics, battery management systems);
- Increase lifetime.

Specific expected impact: Low cost, long lifetime and high energy density batteries by deploying novel materials, chemistries, and cell designs. (Please see **Market, overall expected impact (2.8)**).

IMPACT EXAMPLES:

Example 1: Newly developed materials (membranes, electrodes, electrolytes, catalysts, sealing materials) and macro-homogeneous models for three next generation redox flow batteries produced at prototype level.[81]

Example 2: Vanadium redox-battery technology with high energy efficiency (>80%), suitability for large-scale energy storage, cost efficiency and 30 years long lifespan.[82]

TRL(now) & TRL(2030): Current TRL levels are in the range of TRL 4-5. Innovation actions, allowing wider European deployment, are recommended but also for the few already existing pilot installations to be upscaled by 2030.

2.8.3 Metal-air batteries

Context: Metals with a high energy density are used for metal-air batteries. They comprise of a pure metal anode and a cathode (mainly a porous material coated with a catalytic layer), a separator and the electrolyte. Li-air batteries are most promising among the different metal-air batteries. In contrast, zinc-air batteries are well-established as primary batteries but development as secondary batteries is at a very early stage. Due to cost advantage and high energy density, secondary Zn-air batteries hold high promise as metal-air technology.

Specific challenges:

- Increased efficiency for Li-air and Zn-air batteries, by reliable membranes, catalysts;
- Adequate and continuous power by effective catalytic layers to reduce power lags when not enough air is fed to the cathode;
- Gradual time scaling of capacity to cover longer ranges from kWh to GWh;
- Reduce self-discharge effects that reduce the capacity and operating life;
- Energy density improvements by increasing of efficiency of metal stripping from the anode during discharge and vice versa for plating during charging;
- Improved safety, by avoiding issues related to the use of pure metals as metal electrodes;
- Improved material recyclability.

Specific expected impact: The enhanced power and energy density of the metal-air batteries will allow longer range electrified vehicles and longer battery lifetime of electronic devices.

IMPACT EXAMPLES:

Example 1: Zinc-air batteries with an energy density higher than 250 Wh/kg and 300 Wh/L, and reversibility of more than 1000 cycles at 80 % depth of discharge (DOD), good safety performance and a cost lower than 300 €/kWh.[83]

TRL(now) & TRL(2030): Current TRLs are in the range of TRL 1-3. TRL progression to 6-7 by 2030 can be reached through relevant research and innovation actions.

2.8.4 Organic batteries

Context: Organic batteries represent a promising approach to replace the well-established lithium-ion technology and fulfil the demand for small, flexible, safe and sustainable energy storage solutions. Batteries that use organic active materials feature superior properties in energy storage as well as better resource availability and disposal compared to metal-based and lithium-based batteries. Unlike most of the inorganic materials, organic electrode materials are also more easily compatible with chemistries beyond lithium, including sodium, potassium, magnesium, aluminium and zinc. Additionally, organics can be dissolved (redox flow batteries) or in solid-state, including aqueous or non-aqueous electrolytes, making organic batteries more versatile for a broad type of electrochemical storage devices. Organic chemistry provides great opportunities

for elaborating innovative electrode materials, allowing tailored structures.

Key specific challenges:

- Optimisation and fine-tuning of the redox potential (cathode or anode);
- Maximising the theoretical capacity (reversible multi-electrons reaction);
- Flexibility in use, either to be used as bulk (small molecules) or flexible electrodes (polymers);
- Reduction of electrolyte account in total mass to increase specific energy.

IMPACT EXAMPLES:

Example 1: Organic batteries by replacing the halide part (Br2) with organic electrolytes which have extremely fast electro kinetics: (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (TEMPO) and hydroxylated anthraquinone di-sulphonic acids.[84]

Example 2: Organic redox flow battery based on new organic AQDS (anthraquinone di-sulphonate) at a low cost (< €150 / kWh) and safe 10 kW Energy Storage System (ESS), integrated in an optimised microgrid infrastructure for distributed energy applications.[85]

TRL(now) & TRL(2030): Current TRLs are in the range of TRL 3-4 since only prototype cell forms have been developed; transitioning, via research and innovation actions, to 6-7 by 2030 is recommended.

2.8.5 Materials for large capacity thermo-solar and heat energy storage

Context: Photovoltaics utilise complex multi-materials, deploying high amounts of critical raw materials, whilst they also have costly maintenance to keep efficiency. The storage of thermal energy is more cost effective than storing electrical energy. Heat storage methods involve storing/extracting heat by heating or cooling a storage medium, e.g., liquid or solid without a change in phase. Currently, molten salts are mostly used as a storage medium for concentrated solar power plants. The range of applications extend from grid-scale storage of heat (district heating) to heat for electricity generation (Concentrated Solar Power (CSP)) and power-to-heat-to-electricity. This is currently limited to CSP plants in certain geographical locations due to required direct solar irradiation ; and a relatively lower energy density for storage.

Specific challenges:

- Use of molten salts for long-term heat storage with sequential electricity generation;
- Widening the applications of thermo-solar energy storage beyond residential use;
- Development of novel materials based on phase change materials (PCMs) with higher latent heat.

Specific expected impact: The application of molten salts for long-term energy storage allows to maintain seasonal thermal energy for a quite long periods of time, which has a great potential for the efficiency of solar power plants, independent of the geographical location. The development of alternative organic salts and phase-changing materials will help to reduce the impacts of using lithium halide sorbents, in terms of use of limited resources and maintenance costs.

IMPACT EXAMPLES:

Example 1: Molten salt "once-through" steam generator (OTSG) allowing fully flexible operation of CSP power plants with fast load changes, while bringing system simplification and cost reductions.[86]

Example 2: Materials and devices for latent heat thermal energy storage (LHTES) at ultra-high temperatures of up to 2000°C, based on PCMs with latent heat in the range of 2-4 MJ/kg.[87]

TRL(now) & TRL(2030): The CSP technologies are currently at TRL 7, while the area of efficient formulations, mixtures or combinations of molten salts is at TRL 4-5. The combined technologies are expected to reach levels close to market uptake by 2030.

2.9 Coating Materials and Aerogels

Context: Coatings ensure efficiency and performance of substrates during the required lifetime. Protective coatings are used on surfaces of different nature to avoid corrosion, fouling, icing, and mechanical deterioration in extreme and harsh operation conditions. Aerogels are mainly used in thermal insulation applications due to their outstanding reduced thermal conductivity, their low weight and intrinsic low fire propagation, contributing to improved energy efficiency in buildings and infrastructures.

Market, overall expected impact: Coatings are used in different functions: From protective coatings in industrial and transport applications to advanced functional coatings in aeronautics, building and infrastructure or the decorative applications in furniture, consumer goods and automotive.[88] Aerogels, on the other hand, are materials of great potential in construction, automotive as well as industrial applications.

Coating materials and aerogels address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Manufacturing technologies' (4.1), 'Advanced Materials' 4.4, 'Circular Industries' 4.8, 'Buildings and industrial facilities in Energy transition' (5.4), 'Communities and cities' (5.5), 'Industrial competitiveness in transport' (5.6) 'Food systems' (6.5), and 'Circular systems' (6.7), mainly by the following factors:

- **Performance improvements of critical parts** through advanced coating materials contributing to the control of corrosion, UV light degradation, fouling, adhesion of undesired substances that typically reduce the efficiency of operations in industrial processes and transportation systems;
- **Energy efficiency of buildings and infrastructure** derived mainly from the advanced thermal insulation properties of aerogels;
- **Design for durability and/or design for recyclability**, with contributions to a more circular economy given the range of applications for coatings and aerogels.

Horizontal challenges:

- The circularity-by-design approach when it is required for a combination of coating materials with different and complex application-driven properties (e.g. UV resistance, humidity protection, etc).

SUSCHEM PILLARS – MULTI-KETS:

Innovation in coating materials and the design for durability and/or recycling will be highly supported by **Enabling Digital Technologies (Chapter 4)** including: 'Materials and molecules design: modelling and simulation developments' (4.1.1), and 'Materials and formulations design–integration with process design' (4.1.2).

Within **Advanced Materials**, relevant topics include: 'Composites and cellular materials' (2.1), '3D-printable materials' (2.2), 'Materials for electronics' (2.6) and 'Membranes' (2.7).

RD&I Actions

2.9.1 Coatings with a controlled lifespan

Context: The production of partially or completely removable coating systems represents a circular approach. Coatings, able to degrade or disintegrate with a triggered mechanism under an external stimulus (e.g. temperature, humidity, pressure or presence of chemicals), will potentially minimise the need for solvents but also allow for a controlled coating removal. Primer components, embedded in the material with the ability to degrade under controlled conditions, can also facilitate coating removal for specific applications. In view of this, novel removal technologies and the subsequent material design to target higher coating removal rates is a research interest with a high potential. Ultimately the possibility of alternative surfaces modifications with a "no-coating" approach is also contemplated.

Key specific challenges:

- Designing triggering systems to get a time-controlled coating removal, after the effective lifetime of the product;
- Maintaining durability of the coating systems during its lifetime, without compromising mechanical performance and functionality;
- Facilitating removal of the coating system without leaving any potential residues that may affect the recyclability of the substrate or the application of an additional coating system.

Specific expected impact: Removable coatings technology will not only reduce costs of separation and increase substrate recovery rates but will also extend the life of the coated parts by application of subsequent coatings after complete removal of the previous one(s). Improving recycling of chemical products such as paints and varnishes is foreseen by the EU working document 'Sustainable Products in a Circular Economy - Towards an EU Product Policy Framework contributing to the Circular Economy' that estimates a recycling potential for 27 % of the chemicals in the chemical industry.[89]

IMPACT EXAMPLES:

Example 1: Self-regenerating functional surfaces. By selective disintegration, individual layers of a stack are removed sequentially until all layers have been removed, with the aim of obtaining intact successive functional layers.[90]

TRL(now) & TRL(2030): Technologies with demanding functionalities such as specific triggered and sequential degradation are currently at TRL between 1-3. More research at lower TRL (1-5) would be needed on disruptive concepts on material design for self-regenerating and/or better removable materials. Demonstration activities would be needed to achieve TRL 6-8 by 2030 for efficient removal technologies.

2.9.2 Insulation aerogels: Improving recyclability

Context: Aerogels are materials that combine very low thermal conductivity, low density and in many cases excellent fire resistance. Insulation aerogels, either based on polyurethane (organic), silica-based (inorganic) or alginate (bio-based), are highly efficient insulation systems due to their intrinsic foamed structure with very low thermal conductivity, as well as a high mechanical performance. Silica based aerogels still represent a niche application, considering the overall market for insulation materials in construction, mainly due to high production costs for these silica-based materials (silica aerogel beads, fibre reinforced mats or powder). Overall, for almost any thermal insulation application (building & construction), there is a strong need to develop materials that match the excellent physicochemical properties of aerogels but that also allow sustainable end-of-life solutions.

Key specific challenges:

- Use of building blocks that can be recycled in a low-energy process;
- Scaling up of aerogel processes while maximising the recyclability of aerogel-based systems;
- Develop aerogel systems with enhanced mechanical properties, dust reduction, and overall robustness to be handled on construction sites;
- Integration of aerogels in composite building structures, enhancing compatibility and integration of systems and allowing for an improved performance during the lifetime;
- Enhancing the recyclability of mono-material construction systems using compatible materials that are easy to be recycled without the need for separation and recovery.

Specific expected impact: The use of aerogels as insulation materials can translate into a lower energy consumption for heating and cooling, that could be a profit not only for the building industry, but also for large civil infrastructures; hence contributing to energy efficiency improvements as also outlined by the 2030 Climate and Energy Framework.[91]

IMPACT EXAMPLES:

Example 1: Aerogel-based composite/hybrid nanomaterials for cost-effective building super-insulation systems, with low thermal conductivity values (0.016 – 0.020 W/ (mK)) and very light (bulk density around 0.2 g/cm^3).[92]

Example 2: 40 % energy savings in building refurbishment, reduced installation and maintenance costs with a life span of 50 years by developing a novel cost-effective, durable, industrialised and easy to install composite insulation cladding system, based on a single structured panel with enhanced insulation properties.[93]

TRL(now) & TRL(2030): The use of organic and inorganic aerogels as highly efficient insulating materials in various applications is already at a very mature stage (TRL 7-9). However, demonstration actions at TRL 7-8 specifically dedicated to recyclability are considered necessary. For the case of bio-based aerogel systems, current TRL 5-7 needs to be further developed to reach TRL 8 by 2030.

2.9.3 Functionalised nano-structured materials for active surfaces

Context: The application of nanotechnology on surface chemistry for the development of active surfaces is of increasing interest.[94] Functional nano-coatings can be used for achieving hydrophilic and hydrophobic surfaces for applications such as self-cleaning and antifouling. Self-healing nano-coatings are also of interest as a solution to protect metals from corrosion in harsh working conditions. Smart textiles and textiles with functional finishes, with long-lasting properties and resistance to washing conditions, are also developed using nanofibres and nano-coatings. Nano-active surfaces have also shown applicability in medical applications, to achieve functionalities like enhanced tissue reparation in orthopaedics and implants. Additional options include using nanomaterials derived from biomass, such as lignocellulose, for the development of bio-based nano-active surfaces.[95]

Key specific challenges:

- Improved durability and prevention of surface degradation of nano-coatings during use;
- Mechanical and chemical resistance in severe working conditions (extreme temperatures, pH, salinity, presence of harsh chemicals);
- Surface functionalisation to cope with demanding applications (e.g. medical applications);
- Introduction of bio-based nano-coatings and nanostructures, with potential of additional functionalities.

Specific expected impact: Nano-active surfaces and nano-coatings can have impact on sectors such as biomedical products, transport, energy, consumer goods by the improvement of durability and the introduction of novel functional properties.

IMPACT EXAMPLES:

Example 1: Anti-microbial and anti-biofilm nano-functionalised material used in i) specialty textiles for public areas and hospitals, ii) water treatment membranes, and iii) implantable medical devices. The proposed one-step coating technologies show potential on low-cost, sustainable and safe coating processes and products as well.[96]

TRL(now) & TRL(2030): The development of nano-active surfaces and nano-coatings with special high-end functionalities is still in an early stage of development (TRL 2-4). Research and innovation actions, plus significant demonstration actions need to be developed for these to achieve TRL 6-8 by 2030. As for anti-microbial and hydrophobic nano-coatings, current TRL is at a more mature stage (5-6), but still innovation actions must be deployed to achieve TRL 8-9 by 2030.

2.9.4 Coatings with protective properties

Context: Anti-microbial coatings and paints are of high importance in healthcare settings, public transportation, surfaces in the food processing industry and other industrial settings. Biocidal, anti-fouling coatings are also key to diminish maintenance costs in maritime transportation and industrial applications where biofouling typically reduces processes effectiveness. Self-cleaning and anti-icing coatings are also of high importance for aeronautics to improve efficiency and safety of aircraft operations and to reduce maintenance costs. In addition, anti-icing protective coatings are of high relevance for the renewable energy sector (i.e. wind turbine blades, photovoltaic panels).

Key specific challenges:

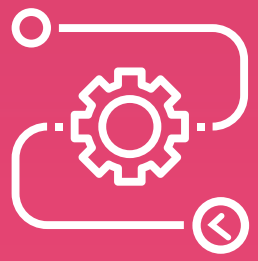
- The ability of a coating to withstand wide temperature range and operating conditions;
- Capability of the coating material to provide the required performance under both static and dynamic conditions.

IMPACT EXAMPLES:

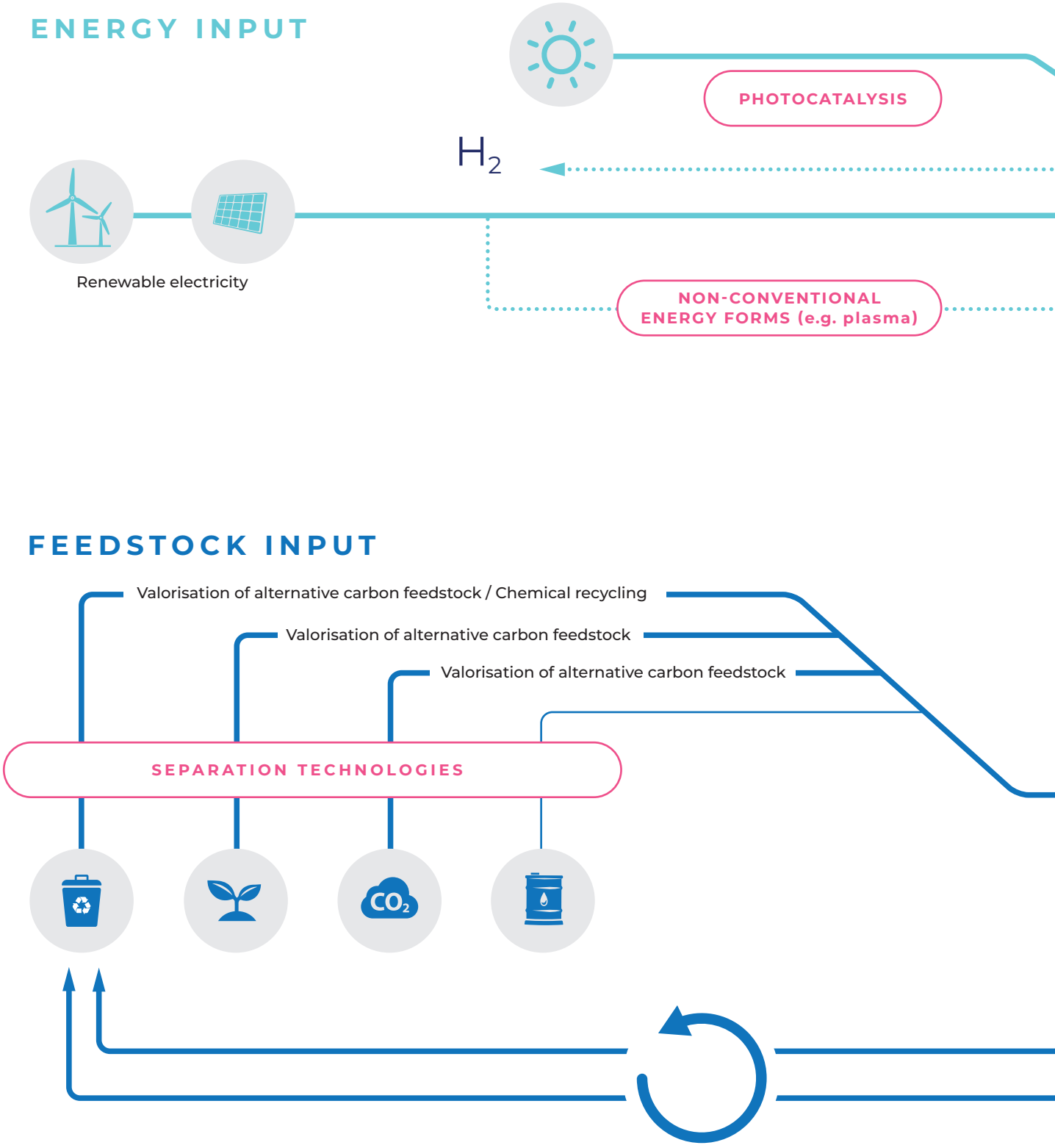
Example 1: Anti-fouling coating, harmless to the marine and human environment. It requires 44-56% less coating than existing solutions and can be removed using a high-pressure water hose, avoiding abrasion or sanding.[97]

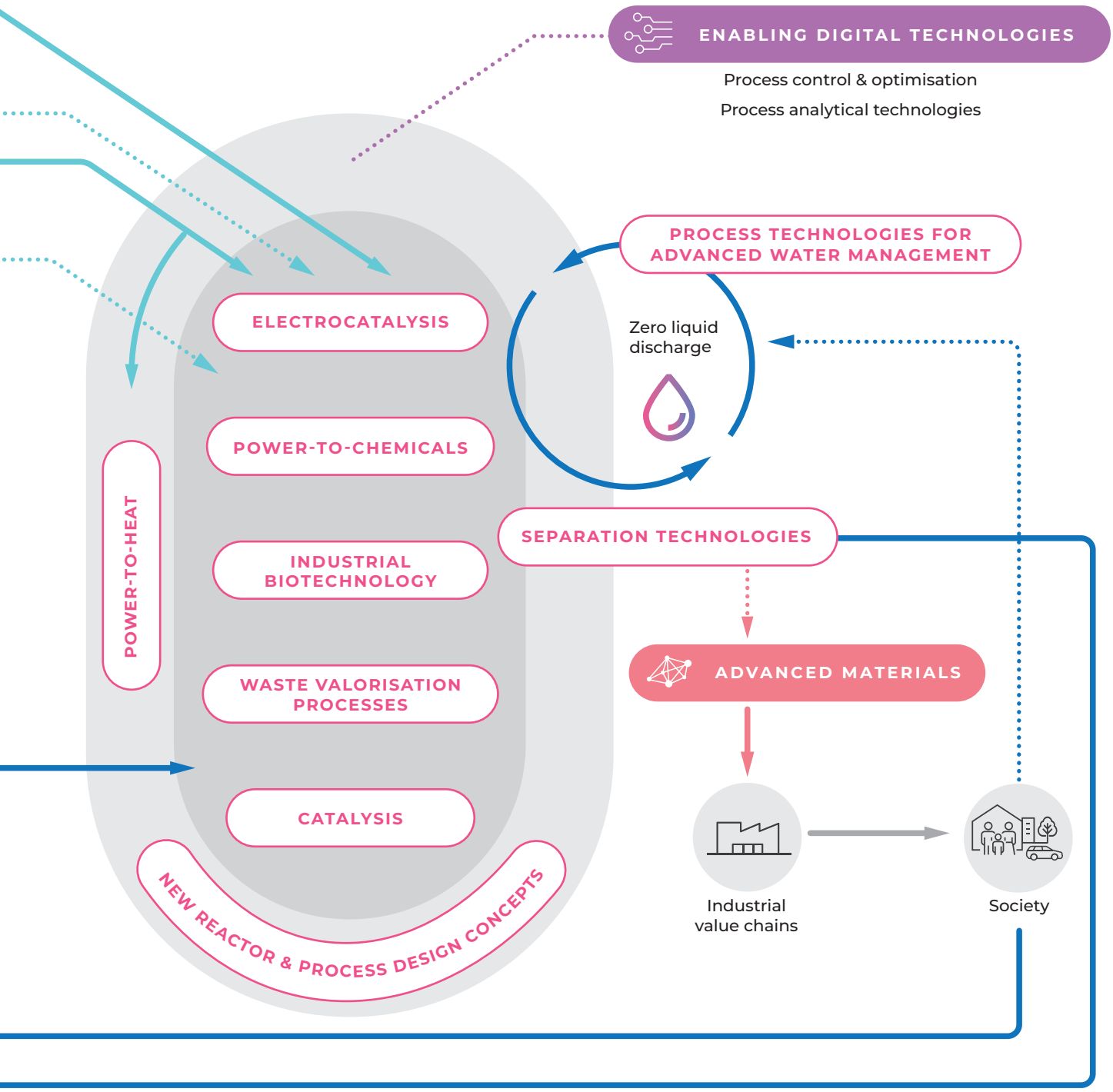
5

ADVANCED PROCESSES



Advanced Processes for energy transition & circular economy




ENABLING DIGITAL TECHNOLOGIES
Process control & optimisation
Process analytical technologies
PROCESS TECHNOLOGIES FOR ADVANCED WATER MANAGEMENT
Zero liquid discharge
ELECTROCATALYSIS
POWER-TO-CHEMICALS
INDUSTRIAL BIOTECHNOLOGY
WASTE VALORISATION PROCESSES
CATALYSIS
POWER-TO-HEAT
NEW REACTOR & PROCESS DESIGN CONCEPTS
SEPARATION TECHNOLOGIES
ADVANCED MATERIALS
Industrial value chains
Society

Advanced Process technologies enable the transformation of raw materials (input) into valuable products (output) of a different chemical structure and composition. They facilitate the production of (solid, gas, liquid) materials and the chemical industry contributes to all industrial value chains through a vast range of end-user products which include transport, food, chemicals, electronics, energy, pharmaceuticals and construction.[98]

The EU chemical industry, including pharmaceuticals, emitted a total of 126 million tonnes of CO_2 equivalent in 2016, down from a total of 325 million tonnes in 1990.[99] This 61.2 % decrease was enabled through energy efficiency and a shift to less carbon-intensive energy sources. At a global level, technical improvements in catalyst and related processes could reduce energy intensity for the top 18 energy intensive large volume chemicals by 20 % to 40 % as a whole by 2050, combining all scenarios.[100] In absolute terms, improvements could save as much as 13 EJ and 1 Gt of carbon dioxide equivalent (CO_2-eq) per year by 2050 vs. a "business-as-usual" scenario.[101]

To reach ambitious targets regarding climate change mitigation and circular economy, disruptive process technologies must be developed in addition to process efficiency options for existing technologies. Novel process technologies will allow increasing the share of renewable energy, including through alternative energy forms and hydrogen. A wide portfolio of products can be produced through a better utilisation of alternative carbon sources such as biomass, including biogenic waste streams, CO_2 (and CO captured from industrial effluents) and waste materials, including plastics waste. As a broader contribution to circular economy, advanced separation and recycling process technologies also allow for critical raw materials and water recovery and reuse. A recent study shows that the ambitious deployment of process technologies to produce major chemical building blocks, utilising low-carbon energy and alternative feedstock (biomass and CO_2), would allow for a very significant CO_2 emission reduction (101 Mt CO_2 /y) for an energy demand of 1 900 TWh and identified that further RD&I actions are needed. Additionally, an exploratory study on chemical recycling, focusing on three plastic waste streams, projected that development of chemical recycling at a reasonably large scale could lead to an annual CO_2 reduction of up to 1.6 Mt for 2030. [102]

Development and innovation in process technologies is critical to the sustainable development of the chemical sector. Hence a portfolio of advanced process technologies and their combination need to be developed, supported by advanced materials innovation and the implementation of enabling digital technologies.

Horizontal challenges

- **Process and plant (re)design** to realise sustainable process intensification, utilisation of alternative feedstock and climate neutral energy sources, supported by advanced sustainability-based process modelling (see **Chapter 4**, **Chapter 5**/Sustainability assessment innovation 5.1);
- **Advanced process control technologies** for optimised production including advanced sensing technologies/ PAT (see **Chapter 4**).

Summary of key priorities for advanced processes to be addressed:

- More **robust and tolerant production processes**, enabling flexibility towards potential specification variations in **feedstock** (e.g. less purified CO_2 streams, integration of different/multiple sources of feedstock in biorefineries), **energy** and **output**;
- **Intensified processes** with **alternative energy forms** such as plasma and microwave technologies for better valorisation of current and alternative types of feedstock;
- **Electrochemical and electrocatalytic processes** including development of new reactor systems, accounting for electrocatalytic electrodes and compact electrolysis cells;
- Advanced **electro-photocatalytic** systems for direct utilisation of sunlight in H_2 production and CO_2 valorisation;
- Advanced **separation technologies**, including membranes (**Chapter 2**), adsorption and integrated reactive separations technologies as well as flexible thermal separation. Applications to vary from upstream to downstream and thus enable recycling (plastics, catalysts, solvents, critical raw materials), and feedstock pre-treatment (e.g. biomass and CO_2);
- **Advanced water technologies** including water reuse and recycling to close the water loop, water symbiosis, decentralised water treatment systems and improved water operations and treatment through data analytics and advanced sensing technologies (**Chapter 4**);
- **Modular** concept for more sustainable continuous production systems for small and medium scale chemical processes, and a competitive approach in new and developing markets. Technical developments include design and realisation of "plug-and-produce" modules equipped with advanced process control (**Chapter 4**);
- **Catalyst** rational design and development (supported by Digital Technologies – **Chapter 4**) for higher selectivity and reduced energy consumption. Novel catalysts should be designed to accommodate more complex and or variable feedstock quality (biomass, waste, CO_2 and light hydrocarbons), and enable integration with separation technologies to reduce the number of process steps. Within the context of process intensification, catalyst and/or reactor 3D-printing could be combined;

- **Industrial biotechnology-based processes** including enzymes and microorganisms engineering, towards the efficient production of fuels, bulk and specialty chemicals but also polymers from new feedstock sources. The increased efficiency of large-scale continuous processes would be the result of bioconversion/upstream and separation/downstream process optimisation (bioreactors and catalyst design, separation technologies and process intensification).

Impact of Advanced Processes innovation – UN SDGs

'Industry Innovation and Infrastructure', via advanced processes to retrofit the chemical industry to become more sustainable, with increased resource-use efficiency and greater adoption of clean industrial processes;

'Responsible consumption and production' through improved process efficiency and utilisation of alternative feedstock, for the sustainable management and efficient use of natural resources, including critical raw materials circularity and the valorisation of waste;

'Climate action', through implementation of advanced processes to significantly lower GHGs emissions;

'Affordable and Clean Energy', via direct improvements in energy efficiency and contributions to the energy transition;

'Clean water and sanitation', through advanced water management, encompassing purification, and recycling;

'Zero Hunger', **'Good Health and Well Being'**, **'Life below water'** and **'Life on land'** by deploying industrial biotech processes to develop food products, novel therapeutics and personalised medicine as well products with positive environmental health implications (e.g. ocean and soil health);

'Decent work and Economic Growth' by achieving higher levels of economic productivity through technological upgrading and innovation in processes.

Advanced Process technologies innovation – relevance to Horizon Europe and other funding schemes

Advanced Processes innovation presents a major contribution to the long-term European policy goals and national priorities. Innovation in advanced processes includes low to high TRLs, with contributions from Academia and Industry, thereby linking with HEU Pillar 1 ('Excellent Science'), Pillar 2 ('Global challenges and European industrial competitiveness'), and Pillar 3 ('Innovative Europe'). Given the thematic approach of Pillar 2, the high relevance on the Horizon Europe clusters and areas of intervention is further elaborated (**Table 5**).

Different instruments and initiatives, beyond Horizon Europe, will be needed for Process Technologies to reach the potential to deliver on ambitious EU targets. The support for upscaling and demonstration, but also 'first of its kind' chemical production plants, will be essential at national and EU levels through instruments such as the Innovation Fund, and Important Projects of Common European Interest (IPCEI).

Table 5: Relevance of SusChem priorities on Advanced Processes with Horizon Europe

Horizon Europe

Pillar 2: Global Challenges and European Industrial Competitiveness

Clusters and Intervention areas

CLUSTER 1: Health	1.1 Health throughout the life course
	1.2 Environmental and Social Health Determinants
	1.3 Non-communicable and rare diseases
	1.4 Infectious Diseases, including poverty-related and neglected diseases
	1.5 Tools, technologies, and Digital solutions for Health & care, including personalised Medicine
	1.6 Healthcare systems
CLUSTER 4: Digital, Industry and Space	4.1 Manufacturing technologies
	4.2 Key Digital technologies
	4.3 Emerging enabling technologies
	4.4 Advanced Materials
	4.5 AI and Robotics
	4.6 Next generation internet
	4.7 Advanced Computing and Big Data
	4.8 Circular Industries
	4.9 Low-carbon and Clean Industries
	4.10 Space including Earth observation
CLUSTER 5: Climate, Energy and Mobility	5.1 Climate Science and solutions
	5.2 Energy supply
	5.3 Energy grids
	5.4 Buildings and Industrial facilities in Energy transition
	5.5 Communities and cities
	5.6 Industrial competitiveness in transport
	5.7 Clean, safe and accessible transport and mobility
	5.8 Smart mobility
	5.9 Energy storage
CLUSTER 6: Food, Bioeconomy, Natural Resources, Agriculture and the Environment	6.1 Environmental Observation
	6.2 Biodiversity and natural resources
	6.3 Agriculture, Forestry and rural areas
	6.4 Seas, Oceans and inland waters
	6.5 Food systems
	6.6 Bio-based innovation systems in the EU Bioeconomy
	6.7 Circular Systems

SusChem priorities: ADVANCED PROCESSES

New reactor design concepts and equipment	●	●						●		●			●		●			●	●						●			●	●	●		●
New reactor and process design utilising non-conventional energy forms.	●	●						●					●		●			●	●					●	●							
Electrochemical, Electrocatalytic and Photo-electrocatalytic processes	●	●						●					●	●	●			●	●					●								
Advanced Separation Process technologies	●	●		●				●		●					●			●	●													
Modular production	●	●																●	●						●							
Power-to-heat	●							●					●	●	●			●	●													
Hydrogen production with low-carbon footprint	●							●		●			●	●	●			●	●					●								
Power-to-chemicals	●							●		●			●	●	●			●	●					●								
Catalysis	●	●						●		●					●			●	●			●			●							
Industrial biotechnology	●	●	●	●	●	●		●		●					●			●	●			●	●					●	●	●		●
Waste valorisation process technologies	●	●		●	●			●		●					●			●	●			●										
Process technologies for advanced water management	●	●	●	●	●	●												●	●													

3.1 New Reactor Design Concepts and Equipment

Context: New reactor, equipment and process design concepts are needed to enable a better utilisation of feedstock (higher selectivity & yield) and /or higher energy efficiency through "process intensification" as well as improve competitiveness. These concepts can find application in chemicals, fine chemicals, polymers, active pharmaceutical ingredients (APIs) as well as fuels production. New equipment design can enable new chemical production routes, for instance through technology change from batch to continuous, which could in turn contribute to improved safety, higher and consistent quality, and lower production costs.

The implementation of new reactor, equipment and process design concepts are essential to techno-economical as well as environmental performance improvements. They enable the integration of climate neutral electricity and the sustainable utilisation of alternative feedstock such as biomass, CO_2 or waste. RD&I actions that can significantly contribute to radical technological progress include reactors and processes tolerant to: feedstock variability, energy fluctuation, electricity fluctuation, batch-to-continuous, microreactor systems, membrane reactors with integrated systems, heat exchange reactors, technologies for heat recovery at low temperature levels, reactors at high temperatures for gas-solid reactions, or 3D-printing of reactors.

Market, overall expected impact: The European vision of a competitive and energy efficient industrial production requires a paradigm shift for the chemical industry, supported by technological breakthroughs in the European chemical industry's transition to resource efficiency and CO_2 emissions reduction.[103] New design concepts and equipment for the full spectrum of chemicals production can reduce the environmental footprint and especially CO_2 emissions, and it will be crucial to reduce dependency on fossil resources. The complex composition of biomass and waste require process flexibility, in regard to feedstock input, whereas renewable electricity integration needs appropriate reactor and process design to respond to electricity intermittency. Additionally, the increasing transition from batch-to-continuous processes is necessary, as part of process intensification, leading to improved process control, process metrics and safety.

Implementing new design concepts and equipment for chemicals, fine chemicals and APIs manufacturing addresses several Horizon Europe (HEU) clusters and areas of intervention: 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Energy supply' 5.2, 'Buildings and Industrial facilities in energy transition' (5.4), 'Clean, safe and accessible transport and mobility' (5.7) and 'Energy storage' (5.9) , 'Bio-based innovation systems in the EU economy' (6.6) and 'Circular systems' (6.7), with additional impact on Cluster 1: 'Health'. Overall impact will be achieved mainly by:

- **Improved robustness and flexibility in the utilisation of alternative feedstock** to produce chemicals, fine chemicals and fuels through tolerant process technologies;
- **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;
- **Introduction of low-carbon energy**, including renewable electricity in chemical processes.

Horizontal challenges:

- Reactor design and engineering to fit specific requirements and maximise process efficiency;
- Maximise synergies with enabling digital technologies with regards to reactor, process and plant design, as well as coordination of processes at different scales.

SUSCHEM PILLARS – MULTI-KETS:

New reactor design concepts and equipment innovation can be integrated with material RD&I actions and enabling digital technologies:

For **Advanced Materials (Chapter 2)**: Processes are essential to the production of all materials and some materials such as 'Membranes' (2.7) are enablers for intensified processes;

For **Enabling Digital Technologies (Chapter 4)**: 'Laboratory 4.0 - Digital R&D' (4.1), 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3, 'Advanced (big-) data analytics and artificial intelligence' 4.4 and 'Coordination and management of connected processes at different levels' 4.8.

Within **Advanced Processes** the relevant topics include: 'Modular production' (3.2), 'Separation

process technologies' (3.3), 'New reactor and process design using non-conventional energy forms' (3.4), 'Electrochemical, Electrocatalytic and Photo-electrocatalytic processes' (3.5), 'Power-to-Heat' (3.6), 'Hydrogen production with low-carbon footprint' (3.7), 'Power-to-Chemicals' (3.8), 'Catalysis' (3.9), 'Industrial Biotechnology' 3.10 and 'Waste valorisation process technologies' 3.11.

RD&I Actions

3.1.1 Tolerant and Intensified Reactors and Processes - feedstock variability

Context: To improve carbon circularity, transition towards alternative carbon feedstock (biomass, waste, CO_2) is becoming increasingly important for the chemical sector. However, alternative carbon sources, such as renewable biomass-based feedstock, can exhibit a high degree of variability in terms of chemical composition. This variability has a strong impact on process control, upstream and downstream purification steps whilst also increasing the need for advanced process analytical technologies within conventional chemical processes. To cope with these challenges, new tolerant chemical processes must be designed that specifically address these issues. This is achieved by systematically taking the variability into account already at the early process design stage. The resulting tolerant processes allow for more flexibility in the utilisation of new types of feedstock.[104]

Specific challenges:

- Experimental and theoretical approaches must be combined to determine adequate models of the feedstock variability;
- Efficient computational algorithms are required to handle the design problem for realistic industrial applications;
- The effect of feedstock variability for a given reaction system must be evaluated by utilising efficient methods for sensitivity analysis.

Specific expected impact: Tolerant processes are an enabler for the transition towards renewable feedstock in the chemical industry.

IMPACT EXAMPLES:

Example 1: The consideration of variability in the feed composition at the reactor design stage reduced the number of temperature constraint violations considerably (from 43 % in the conventional reactor to 3.4 % in the tolerant reactor).[105]

Example 2: 95 % reduction in GHG emissions by developing a process for converting agricultural residues into bioethanol using process-integrated enzyme production for simultaneous conversion of cellulose and hemicellulose into ethanol as part of an energy-efficient process design. This process overcame technological challenges to arrive at a commercially viable basis.[106]

TRL(now) & TRL(2030): There are already (very few) tolerant processes established at TRL 7-9. However, generally applicable design procedures for tolerant processes that are transferable to other examples are not yet available and standardised and are currently still at low TRL (1-4). Thus, more fundamental work and experimental validation is required so that higher TRL (5-7) can be achieved by 2030.

3.1.2 Tolerant and Intensified Reactors and Processes - energy fluctuation

Context: Energy transition to renewable sources calls for an innovative design of chemical reactors and processes which are highly tolerant to fluctuations connected to energy supply. Of great relevance are Power-to-X concepts, where excess power at peak loads is used to synthesise chemical energy carriers for energy storage. While a conventional chemical plant is typically operated at the most economical steady state operation point, a Power-to-X plant needs to adapt to the current (fluctuating) energy supply. Such load-flexible plant operation causes severe dynamic effects which is a great challenge for both reactor and process design as well as for process control.

Specific challenges:

- Intensified chemical reactors, which allow for a very fast and safe dynamic transition of different load levels while maintaining the desired product quality specifications and plant safety requirements;
- Selection of suitable materials and structural geometries of the chemical reactor and identification of a robust catalyst regarding deactivating influences;
- Advanced process control systems which can cope with a highly dynamic process operation;
- Dynamic operation of integrated chemical sites e.g. resource efficiency of one-pipe systems.

Specific expected impact: Intensified reactor and process design and control with improved tolerance to energy fluctuations enable economically efficient decentralised, stand-alone plants (often small- to medium-scale) close to the energy source which is especially significant for the synthesis of chemical energy carriers.

IMPACT EXAMPLES:

Example 1: 85 % reduction of carbon footprint in an innovative Power-to-Gas storage plant supplied exclusively from the nearby wind and solar installations, paving the way for an integration of Power-to-Gas storage into flexible energy supply and distribution systems with a high share of renewable energy.[107]

TRL(now) & TRL(2030): The technology of Power-to-Gas plants has been demonstrated for a steady state operation at commercial scale, but with little tolerance to fluctuations.[108] Intensified, stand-alone systems with high tolerance to fluctuations are currently at TRL 4-5 but should achieve TRL 6-9 by 2030.

3.1.3 Impact of electrification on reactor design

Context: In the context of the energy transition, the electricity market experiences a structural change by integrating an increasing share of renewable energy such as wind, and solar, leading to a fluctuating power supply. To save temporal excess of energy, large scale storage systems are needed. In this context, the interest in Power-to-Gas technologies has increased as it offers the possibility for large scale energy storage, e.g. in the form of methane. Parallel to the Power-to-X concept, also the direct use of electrical energy for technological purposes in chemical plants is pursued. It can be used as Power-to-Heat for preheating process media instead of using traditional heat carriers or as a source of energy for chemical conversions. A broad availability of affordable, climate-neutral electricity will be a driver for new generation of more efficient electrically driven reactors and processes.

Specific challenges:

Specific challenges regarding reactor design are:

- Effective energy distribution in the reactor volume and avoiding of fouling near the energy supply spots are very important;
- New design concepts must consider limitations resulting from the available materials for reactor design and safety aspects, especially for high temperature and high-pressure applications.

Specific expected impact: Electrification of chemical reactors, especially those used in bulk chemicals production can significantly contribute to the reduction of the GHGs emissions. Electrical heating based on climate-neutral electricity can contribute to reduce significantly CO_2 emissions from heating.

IMPACT EXAMPLES:

Example 1: Large-scale production of hydrogen through steam reforming directly produces CO_2 as a side product. In addition, the heating of reactors through fossil-fuel burning contributes further CO_2 emissions. Adoption of this alternative approach could affect CO_2 emissions by up to approximately 1 % of global emissions.[109]

Example 2: CH_4 conversion of up to 29.4 % using one heating element at 900 °C through the development of an electrically heated catalytic reformer for dry reforming of methane and reverse water-gas-shift reaction. Thermodynamic conversion and high space-time-yields have been achieved with the developed electrically heated and catalytically coated foils.[110]

TRL(now) & TRL(2030): Reactor design tolerant to electricity fluctuations has been achieved at TRL 3. Therefore, innovation and demonstration actions are recommended by 2030.

3.1.4 Batch-to-continuous: Flow Chemistry

Context: Reactions can be run in a continuously flowing stream of reactants, a production mode that is well known from the large-scale production of bulk chemicals. Compared to batch reactors, continuous flow reactors allow the management of reactions with significantly higher reaction enthalpy. In turn, temperature can be raised so the residence time can be decreased compared to batch operations. Since it is easy to operate at elevated pressures, reaction temperature can be raised above the solvent's boiling point. Time for mixing of reactants is very short which is beneficial for fast reactions. Multistep reactions can be easily arranged in a continuous sequence. This can be especially beneficial if intermediates are unstable, toxic or sensitive to air. The further drivers for application of flow chemistry are higher selectivity and yields, as well as easy automation regarding process control. Reactions in flow can be run in microreactors. However, usually capillaries with diameter up to several millimetres are used, at least in the laboratory development stage. On the market various set-ups for testing reactions in flow are available, most of them use capillaries. A number of reactions have been studied and the potential of this technology has been shown, e.g. for fast metalloorganic reactions.

Specific challenges:

- Evaluation of experimental data is usually based on the simplified assumption that there is no residence time distribution (plug flow) and no temperature gradients in the reactor. These assumptions have a significant impact on scale-up;
- Rational scale-up of continuous flow reactors, accounting for temperature spikes that can lead to an almost adiabatic temperature rise;
- Develop approaches for fast determination of kinetics. For this purpose, characterisation of fluid hydrodynamics and heat and mass transfer is necessary. This should be the foundation for rational scale-up which can be applied to microreactors but also other reactor types like cascades of continuous stirred tank reactors (CSTRs), tubular reactors or multicell reactors;
- New scalable designs of clogging resistant continuous flow reactors for process intensification. With this respect, two concepts should be studied: "end-to-end" and "flow-when-needed". In the "end-to-end" concept all synthesis and separation steps of a multistage process are performed in flow, in the process intensified equipment. In this approach there are strong synergies with 'Modular production (3.2)'.

Specific expected impact: Flow chemistry can have a significant impact on the chemical and pharmaceutical industry. The main drivers for implementation are the improved safety, higher and constant quality, and competitiveness. There are already single examples of the commercial or semi-commercial units for the syntheses in flow, e.g. safety critical reactions[111] or "on-demand" production of pharmaceuticals.[112]

IMPACT EXAMPLES:

Example 1: Shifting from batch-wise processes comprising many separate unit operations to highly integrated and flexible catalytic continuous flow processing, applicable to low-to-medium-scale chemical and pharmaceutical production. Continuous flow processes resulted in superior performance, advantageous for small-to-medium-scale production.[113]

TRL(now) & TRL(2030): Reactions in continuous flow reactor are currently at TRL 4 for fine chemicals. More demonstration activities to show the systematic scale-up of this technology (from the laboratory to the pilot scale) as well as techno-economic evaluation of the different concepts together with the development of suitable business models would be beneficial by 2030.

3.1.5 Microreactor systems

Context: Micro process engineering is a technology for performing chemical (microreactors-MRT) or physical processes (unit operations) inside channels with effective diameters of less than 1 mm (microchannels) or other structures with sub-millimetre dimensions. The processes are usually carried out in continuous flow mode. The range of the channel diameters is also frequently extended up to 10 mm. For the modules with larger channels, also the term millireactors is frequently used. The unique advantages of micro-structured reactors are enhanced heat transfer and efficient mixing of reactants during very short times. In case of multiphase reactions an enhanced mass transfer is important. The good heat transfer ability of microreactors allows precise temperature control, in particular for highly exothermic reactions. Moreover, microreactors allow to perform in a stable and safe manner reactions that can't be handled in the classical reactors.

Specific challenges:

- Overcome the limitation of microreactors to sensitivity to fouling and clogging. Solutions are needed for monitoring of fouling and prevention of clogging, e.g. by a reactor design or clean-in-place approaches;
- Research and demonstration activities to scale up this technology. Studies on model-based scale-up are needed, especially to control process parameters to avoid runaway reactions. The prerequisite for model-based development is linked with the comprehensive characterisation of the module;
- Suitable sensors that can be integrated in microreactors for online analytics;
- In many relevant reaction systems solid particles are present either as a reactant or product. Therefore, scalable concepts for solids handling are necessary. The same is valid for application of the MRT for electro- and photochemistry;
- To build MRT-based plants, concepts for integration of microreactors with process intensified separation technologies are needed. This topic has a large overlap with the topic 'Batch-to-continuous: Flow chemistry' **(3.1.4)** and 'Modular production' **(3.2)**.

3.1.6 Membrane reactors - integrated systems

Context: Membrane reactors are multifunctional reactors, applicable to performing and controlling a chemical reaction and simultaneously controlling the feed of one of the reactants and/or the removal of one of the products. Membrane reactors can be applied for performing reactions in gas- or in the liquid phase. Application of feed control allows to control reaction rate which is very important for performing highly exothermic reactions in a safe and stable manner. Furthermore, by means of the accurate control of the temperature also selectivity could be improved. Several reactions have been studied in this type of membrane reactors, e.g. oxidations, oxidative dehydrogenations, and aromatisation reactions. Alternatively, membranes could be used for in situ product removal, overcoming limitations resulting from the thermodynamic equilibrium of a reaction/process.

Specific challenges:

The major obstacle for implementation of this concept is the availability of suitable membranes that exhibit sufficient selectivity, permeability and stability (incl. inorganic (ceramic or metallic) and polymer membranes). Detailed discussion of challenges and potential solutions is given in the section 'Separation technologies' **(3.3)** and 'Membranes' **(2.7)** under the Advanced Materials chapter.

3.1.7 Heat-exchanger reactors (HEX)

Context: Heat-exchanger reactors bring the advantage of using existing manufacturing technologies and capabilities. It has commercial potential since it is an easy way to replace the economy of scale by the lower costs of manufacturing in series. In this sense it shares the concept of modular production. Heat exchanger reactors have the largest potential for application for liquid-phase reactions. Therefore, they have a large potential for the transfer of the reactions from batch to continuous operation mode **(**see **3.1.4)**. Depending on the materials and manufacturing technology they can be also used for gas-phase reactions. After adaptations, they can be also used for heterogeneously catalysed reactions. By means of advanced heat exchangers, e.g. fin-plate heat exchangers reactors, advanced heat removal potential could be realised. They build an intermediate stage between the micro-structured **(**see **3.1.5)** and multi-tubular reactors. Larger channels than in the microreactors have the advantage of improved robustness against clogging.

Specific challenge:

A lack of design basis bring the need for experimental studies to develop correlations describing heat and mass transfer in different types of channels of commercially available heat exchangers.

3.1.8 Reactors for high-temperature gas-solid reactions

Context: High-temperature gas-solid reactions are used to produce several high-value products such as catalysts and pigments or in catalytic pyrolysis of biomass. Gas-phase conversions exhibit the potential of generating less process waste when compared to liquid phase reactions. On the other hand, the high temperatures applied cause a large energy demand that needs to be optimised. The use of smaller particle sizes also contributes to the need for development of new reactor types.

Specific challenge(s):

- Conversion of the feedstock to the desired particles morphology, e.g. preventing of particle agglomeration;
- Scale-up of reactor design is challenging. Due to the high temperatures and frequently also harsh reaction conditions, there are limited possibilities for the online measurements. Scale-down is not easy since the heat loss increases dramatically.

3.1.9 Reactors customisation: 3D-printing

Context: Additive manufacturing gives the possibility to produce highly specialised three-dimensional structures with nearly no limits in the geometric complexity. Furthermore, additional functionalities such as heating/cooling or catalytic activity can be integrated directly in the component. That way, the technical realisation of a new generation of tailor-made reactors and process components with significantly higher efficiency is possible. Before the potential of this new concept can fully be exploited for applications in the chemical process industries, there is still a significant need for R&D. In this regard, theoretical methods and models (e.g. correlations and design rules) have to be established. Furthermore, demonstration projects in technical case studies under industrial relevant conditions must be carried out.

Specific challenges:

- Production of the 3D-structures (e.g. adaptation for a broad material basis);
- Surface functionalisation (e.g. with catalytic active material);
- Characterisation of the structures in terms of heat and mass transport properties;
- Concepts for the technical implementation in industrial processes;
- Integration of additional functions (e.g. sensors).

Specific expected impact: Additively manufactured catalytic structures can achieve a significant impact on reducing CAPEX/OPEX and increase energy- and resource-efficiency of chemical processes.

IMPACT EXAMPLES:

Example 1: Using structured catalyst carriers instead of randomly packed fixed bed reactors, it is possible to enhance the heat transport, especially for low and/or fluctuating superficial velocities. Furthermore, by optimising the wall contact of the structure, the overall heat transport can be increased up to 300 %. This can lead to lower hot spot temperatures and slower catalyst deactivation, which allows for significantly extended catalyst service lifetime.[114]

Example 2: In multiphase applications, the liquid distribution within structured packings can be enhanced by the usage of optimised unit cell geometries. With such additively manufactured geometries, an improved liquid distribution up to a factor of two is realisable, thereby increasing the interaction between liquid, gas and solid phase and consequently enhancing the specific reaction rate.[115]

TRL(now)&TRL(2030): The generation of tailor-made reactors through 3D-printing is currently at TRL 4, thus more demonstration activities at higher TRL (6-8) need to be achieved by 2030.

3.2 Modular Production

Context: Modular production encompasses highly adaptable production lines to enable flexible and efficient production of small volumes of products that can be tailored to customer demands. It will also enable decentralisation of production (e.g. biorefining).

Market, overall expected impact: The chemical sector, especially in Europe, is facing increased market competition, whilst at the same time needs to increase process flexibility and reduce volumes of products with a faster supply-demand response. Modular production can contribute to improve customised, flexible and decentralised production with a potential for use in a wide range of chemical products.

Consequently, modular production addresses several **Horizon Europe (HEU) clusters and areas of intervention:** 'Key digital technologies' 4.2, 'Circular Industries' 4.8, 'Low-carbon and Clean Industries' 4.9 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) mainly by:

- **Improved resource and energy efficiency** by achieving efficiently shorter production cycles;
- **Improved flexibility in products customisation** with a faster response to supply chain / customer demands, creating opportunities for new business models enabled by digital technologies;
- **Enable decentralised production** for biomass and waste valorisation in the context of a more circular economy.

Horizontal challenges:

- Adapt Process Analytical Technologies (PAT) for modular production, to support process control, automation and predictive maintenance and process coordination;
- Standardisation of modular production concepts.

SUSCHEM PILLARS – MULTI-KETS:

Modular production innovation will have impact on **Advanced Materials (Chapter 2)** production, especially '3D-printable materials' (3.2) and 'Bio-based chemicals and materials' (2.3).

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable modular production, in particular 'Process Analytical Technologies (PAT)' 4.2.

Modular production is expected to be further impacted by other **Advanced Process Technologies (Chapter 3)** and especially on processes related with the integration of alternative feedstock: 'Tolerant and intensified reactors and Processes tolerant to feedstock variability' (3.1.1), 'Separation process technologies' (3.3), 'New reactor and process design utilising non-conventional energy forms' (3.4), 'Electrochemical, electrocatalytic and electro-photocatalytic processes' (3.5), 'Power-to-Chemicals' (3.6), 'Industrial biotechnology' 3.10, 'Waste valorisation process technologies' 3.11 and 'Process technologies for advanced water management' 3.12.

RD&I Actions

3.2.1 Modularised production plants

Context: Modularisation can increase flexibility in terms of capacity (e.g. by numbering-up or parallelisation), product mix (e.g. by exchange of reaction or downstream processing modules following a plug and produce), feedstock and site (e.g. mobility of modules). The core concept of modular production includes the physical modularisation of the apparatuses for reactions as well as upstream and downstream processing, and affect the plant design and planning, infrastructure, utilities, analytics and automation. Modularisation of the production plants should be integrated in suitable supply chain and business models. Therefore, development of new modular plants needs a holistic approach.

Specific challenges:
Challenges in modular production relate to equipment for modular production, operation of modular plants, and methods and tools.

Equipment for Modular Production:
- Improved flexibility of equipment (e.g. for a broad applicability and parameter range);
- Intelligent equipment / modules (e.g. self-x functionality, integrated sensors for improved process information, link to external data for optimisation);
- Smart equipment in intensified up- and downstream processing with additional control opportunities;
- Miniaturisation and cost reduction of equipment (especially sensor technology, automation, process control, switch cabinets);
- Small and smart laboratory equipment for measuring and optimising intensified process steps.

Operation of Modular Plants ("Plug & Produce"):
- Remote operation (safety and authority engineering aspects);
- Modular automation in continuous operation as well as process orchestration layer;
- Expand to new process areas (e.g. decentralised biorefineries);
- New business concepts (e.g. life cycle management, rental, maintenance).

Methods and Tools:
- Life Cycle Analysis for modular plant concepts and their operating models (e.g. rental of modules, shared use, shared maintenance);
- Economic analysis tools to quantify the flexibility of modular plants as well as the benefit of a split in investments;
- Modelling of process equipment assemblies (PEAs) and the full modular plant (digital twin);
- Modelling of process steps and application of advanced process control for online optimisation.

Engineering guidelines and standardisation:
- Engineering guidelines and standardised processes (e.g. modular process equipment assemblies, concepts for scale-up and scale-up stages);
- Accelerated authority approval for modular flexible plants, and development of international standards (e.g. joint developments).

Specific expected impact: Modularised production plants to achieve a significant impact on reducing production costs, design effort, time-to-market, carbon footprint, logistics effort, CAPEX/OPEX and increasing efficiency (e.g. less processing steps, less solvent and energy consumption) and improving space-time-yield.

IMPACT EXAMPLES:

Example 1: Up to 20 % reduction of OPEX, up to 40 % reduction of CAPEX and 50 % reduction in time-to- market through the development and implementation of a modular, continuous production technology using novel, intensified equipment and processes in a standardised, container-based manufacturing environment for low to medium scale production.[116]

Example 2: Development of a new concept for modular production for the chemical industry using adaptable plants with flexible output, generating an economic impact of €10 million/a (cautiously optimistic) to €30 million million/a (optimistic) by direct exploitation and up to €800 million/a (very optimistic) by indirect exploitation via technology transfer.[117]

TRL(now) & TRL(2030): Modular production plants have achieved a TRL5, with some pilot and demonstration units already designed and constructed (TRL 5-7). Further developments are needed, in particular regarding downstream and upstream processes and PAT. More demonstration activities focusing on demo to industrial production scale at higher TRL (7-9) need to be achieved by 2030.

3.3 Separation Process Technologies

Context: Separation technologies are of crucial importance for large-scale chemical and biotech processes, contributing more than 40 % of capital and operating costs.[118] Advanced separations and further innovation in this area are required to significantly reduce such costs. These technologies encompass, amongst others, integrated systems where tailor-made membranes (e.g. for catalysis and separation) and membrane reactors can be coupled with continuous processes with high potential for in-situ recovery and re-use of resources. Other advanced separation technologies include reactive and/or enhanced distillation, adsorption technologies, advanced filtration systems, utilisation of alternative solvents or colloidal separation and concentration.

Market, overall expected impact: Mature separation technologies represent up to 50 % of the energy consumption in chemical plants, being very energy intensive[119]. Advanced separation technologies contribute to further improving the energy and overall efficiency of chemical and biotech processes and the development of alternative production routes. They are also enablers for the utilisation of alternative carbon sources such as biomass, CO_2, or waste (incl. non-organic waste valorisation), contributing to the development of a circular economy.

Separation technologies address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Clean, safe and accessible transport and mobility' (5.7) and 'Energy storage' (5.9), 'Industrial competitiveness in transport' (5.6), 'Seas, oceans and inland water' (6.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) mainly by:

- **Improved resource and energy efficiency in chemicals production**, including platform chemicals, fine chemicals, or polymers. This to be achieved by improving reaction control, selectivity and purification efficiency (upstream and downstream) and increasing resource and energy efficiency by recovering reaction substrates, catalysts, and solvents, at potentially lower energy input;
- **Improved efficiency in gases production and/or gas mixtures separation/purification prior to valorisation:** Efficient production of gases (e.g. H_2)[120] or the valorisation of gases (e.g. CO_2)[121] to chemicals or fuels;
- **Enabling the valorisation of alternative carbon feedstock:** the downstream and/or upstream application of advanced separation technologies enable the sustainable production of chemicals and fuels from biomass, CO_2 or waste;
- **Enhancing the recycling of plastics:** the chemical recycling of plastics will require the development of new separation technologies, in order to remove impurities in the waste streams and treat multi-layered plastics or to separate fillers (glass or carbon fibres, inorganic pigments), with a key contribution to circular economy;
- **Recovery of valuable materials such as metals or critical raw materials (CRMs) from concentrated waste** (e.g. WEEE), **industrial streams or water sources** (e.g. wastewater, saline water and brine) will allow for circularity. For instance, the recovery of Platinum Group Metals[122], or other metals for electric vehicles, energy storage and generation such as Rare Earth elements, cobalt or even lithium[123] would contribute to secure the supply of strategic raw materials for EU industries;
- **Water treatment and seawater desalination** at lower energy requirements.

Horizontal challenges:

- Reduction of energy required for advanced separation operations (upstream & downstream);
- Integration of more compact and robust systems (including antifouling and overall enhanced lifecycle), contributing to less capital-intensive system design;
- Performance improvements, beyond energy-efficiency: processing speed, and improved process metrics (yield, & selectivity).

SUSCHEM PILLARS – MULTI-KETS:

Advanced separation technologies will have impact on **Advanced Materials (Chapter 2)** production including from alternative feedstock, whereas 'Membranes' (2.7) will enable advanced separation technological developments.

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable modular production, in particular 'Laboratory 4.0 - Digital R&D' (4.1), 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3 and 'Predictive maintenance' 4.5.

Advanced separation technologies are expected to impact other **Advanced Process Technologies (Chapter 3)** and especially on processes related with the integration of alternative feedstock (CO_2, biomass, waste): 'Tolerant and intensified reactors and Processes tolerant to feedstock variability' (3.1.1),

'Membrane reactors - integrated systems' (3.1.6), 'Modular production' (3.2), 'Electrochemical, electrocatalytic and electro-photocatalytic processes' (3.5), 'Power-to-Chemicals' (3.6), 'Hydrogen production with low-carbon footprint' (3.7), 'Catalysis' (3.9), 'Industrial biotechnology' (3.10.2, 3.10.3), 'Waste valorisation process technologies' 3.11 and 'Process technologies for advanced water management' 3.12.

RD&I Actions

3.3.1 Membranes integration in continuous processes

3.3.1a. Integrated separation and catalytic processes

Context: Integrating reactor-catalyst-separation design in continuous conversion processes, can involve robust membrane reactors that combine separation and catalysis in one unit. The catalyst may be deposited on the membrane surface (gas phase reactions) or dispersed in a liquid medium (membrane slurry reactor). These membranes can thereby, increase efficiency when compared to conventional reactors. In addition, catalytic membrane reactors allow for integrated processes, for energy and resource efficiency by improving the process metrics and catalyst recycling.[124] Selective transport properties of the membranes can also be used to improve the reaction kinetics by selectively removing products and by-products from the reaction mixture and/or the selective supply of reagents.

3.3.1b. Separation applications (concentrated & diluted conditions)

Context: Innovative separation technologies find a large variety of applications even when decoupled from catalytic conversions (e.g. membrane distillation crystallisation for brine mining, separation membranes for chemicals refining). For example, membrane distillation allows for water treatment, the recovery of compounds (metals or organics), or the treatment of industrial waste streams.

Specific challenges (1a & 1b):

- Overall improvements in energy efficiency for demanding applications; for example, water treatment under high salinity and organic loading requires high energy input;
- Fouling of the membrane is a common materials design issue but also process innovation challenge that needs to be tackled in the development of membrane reactors;
- Reduction in CAPEX and OPEX linked with the fabrication and operation of membrane reactors, where current modelling and simulation remains a challenge.

Specific expected impact: Integrated membrane-based continuous separation and catalytic conversions as well as process innovation for more efficient separation applications to achieve significant impact on reducing CAPEX/OPEX, CO_2 emissions as well as energy and cost intensity in a plethora of applications.

IMPACT EXAMPLES:

Example 1: 20 %-30 % lower CAPEX and OPEX, 50 % reduced energy intensity, 60 % lower CO_2 emissions and 10-15 % higher yield of the direct catalytic conversion of methane into ethylene through a novel membrane reactor allowing for process intensification.[125]

Example 2: A multifunctional catalyst integrated in an electrochemical cell enabled for a scalable technology of CO_2 valorisation, increasing reaction metrics (CO_2 per-pass conversion >85 %), energy efficiency (> 85 %) and net specific energy demand (< 6 MWh/t CO_2).[126]

Example 3: Membrane Distillation Crystallisation enabled a sustainable wastewater treatment process by creating additional value streams to offset water treatment costs, using lower operating temperatures (40-60 °C), and lower hydrostatic operating pressures.[127]

TRL(now) & TRL(2030): For some application areas (e.g. water removal for hydrocarbon synthesis , H_2 production, water treatment, etc.) there are some technologies currently at TRL 5. For those, more demonstration activities at higher TRL (6-8) need to be achieved by 2030. More fundamental research at lower TRL (1-5) would be on exploring new designs and concepts for membranes and membrane reactors to reduce further: energy consumption, CAPEX/OPEX, and emissions while generating new products from alternative carbon feedstock.

3.3.2 Continuous reactive separation processes

Context: Continuous reactive separation processes combine reaction and separation into a single unit and may also include the deployment of membranes.[128] This improves process metrics and reduces downstream purification intensity leading to high-efficiency systems with sustainable engineering attributes. Overall, some of these benefits are realised by using reaction to improve separation while others are realised by using separation to improve reactions—the maximum effect being achieved when both aspects are important.[129]

Specific challenges:

- Developing continuous product separation/in-situ recovery for product sensitive or equilibrium reactions;
- Controlled (labile) reagent/substrate addition with solvent recovery;
- Continuous recovery and re-use of excess reagent for slow reactions/kinetic enhancement;
- Continuous recovery of catalysts (e.g. homogeneous catalysts (nanofiltration), heterogeneous catalysts or biocatalysts (ultrafiltration)) for intensified reactor concepts and as alternative to catalyst heterogenisation.

Specific expected impact: Continuous reactive separation processes can achieve a significant impact on reducing CAPEX/OPEX and energy and resource-intensity costs.

IMPACT EXAMPLES:

Example 1: Novel membrane electrolysis, employing an integrated continuous fermentation coupled with simultaneous organic acid removal, allowed the conversion of Municipal Solid Waste (MSW) to intermediate chemical products at high yields and selectivity (e.g. lactic acid or succinic acid, both being critical platform chemicals).[130]

Example 2: Fermentation and conversion processes with coupled recovery in biofilm reactor systems to convert agro- waste streams into biobutanol, a promising biofuel, valorising 50 % of the unavoidable and under valorised agro- waste as feedstock, diverting up to 45 million tonnes of food waste from EU landfills, preventing 18 millon tonnes of GHGs emissions and saving almost 0.5 billion litres of fossil fuels.[131]

TRL(now)&TRL(2030): The development of reactive separation processes to produce or recover value added chemicals from waste or biomass has achieved a TRL 5, more R&I on demonstration and optimisation of separation processes from waste or biomass at TRL 6-8 needs to be considered by 2030. Reactive separation for metal recovery or water treatment has achieved TRL (1-5), while other reactive separation processes for these applications have already achieved a TRL 5. Similarly, for membrane-based processes (3.3.1), fundamental research will also allow for further improvements and new production routes, including the more efficient valorisation of alternative feedstock.

3.3.3 Integration of alternative solvents for advanced separations

Context: Alternative solvents include amongst others supercritical CO_2, supercritical fluid chromatography, deep eutectic solvents (DES), or ionic liquids for upstream and downstream applications, with benefits of low exposure toxicity and flammability whilst often allowing for solvent recycling and re-use.

Specific challenge(s):

- Supercritical CO_2, a mature technology, presents high CAPEX and OPEX costs with high pressure operation requirements and challenges in some continuous flow processes. Process innovation to establish a larger applications portfolio where supercritical CO_2 brings significant sustainability improvements should be explored further;
- Supercritical fluid chromatography, ionic liquids and DES envision more fundamental research for a decrease in OPEX costs. Furthermore, DES and ionic liquids present mass and heat transfer limitations for some applications and also need better understanding with regards to toxicity and their effects on (bio)catalytic reactions;
- Further research on other novel alternative solvents is also recommended for advanced separations applications, providing sustainability metrics improvements.

3.3.4 Adsorption technologies for upstream and downstream applications

Context: Adsorption technologies have already achieved a wide range of applicability in separation processing steps (e.g. upstream or downstream physisorption or chemisorption for gas separations), with variability in energy efficiency across applications. The development of materials with higher adsorption capacity for selectivity can broaden the scope of adsorption, which could be seen as an alternative or a complement to distillation. Adsorption could become more competitive than absorption with amines for CO_2 capture.

Specific challenge(s):
There is a need to integrate materials and process innovation, addressing the relatively limited variety and flexibility of scalable and robust adsorbents, but also the physisorption, and chemisorption requirements whilst designing processes that also contribute to address energy and resource (including the adsorbent) efficiency. It is notable that adsorption technologies often suffer from high OPEX costs, mainly driven by the regeneration of the adsorbents.

3.3.5 Distillation intensification

Context: Distillation, being the most commonly used separation technique in the chemical industry, is a crucial component of process intensification to boost the efficiency of a process plant. In order to reduce the high energy and capital cost requirements, a specific focus on further intensification of distillation technologies such as heat integration distillation columns (HIDiC), dividing wall columns (DWC), high gravity (RPB), and (bio) reactive distillation (e.g. enzymatic) is required.[132]

Specific challenge(s):
- Compact, easy to operate, energy efficient and cost-effective multi-component systems;
- Distillation system configuration, design, modelling and control issues;
- Reactor distillation constraints on thermodynamic requirements, overlapping of reaction and distillation operating conditions and availability of catalyst with sufficient longevity.

3.3.6 Advanced filtration technologies

Context: Advanced filtration technologies are needed for more efficient separation across sectors, including processing water, waste and biomass.

Specific challenge(s):
Overcome the currently restricted use due to limited choice of materials set; combined materials and process innovation is recommended to advance further.

3.4 New Reactor and Process Design Utilising Non-conventional Energy Forms

Context: Alternative energy forms such as ultrasound, microwave, plasma, light, or high gravity are non-conventional, non-contact energy sources that create the possibility for new and flexible process windows in flow reactors. Energy sourced from non-conventional energy forms is more efficient in terms of being applied exactly where it is needed, as well as reducing reactions times, facilitating synthesis automation, thus promoting also its use for more sustainable chemical processes.

Market, overall expected impact: These alternative energy forms have been identified as novel key process-intensification concepts. Additionally, they would contribute to the transition from batch to continuous micro and milli- flow processes for fine chemicals and possible application at larger scales.
The implementation of alternative energy forms which are electricity intensive would contribute to the integration of renewable energy into chemical production. Some alternative energy forms such as plasma and microwave can also contribute to the valorisation of waste, biomass and CO_2 as feedstock. To maximise impact major knowledge gaps have to be addressed with regard to the mechanisms underlying alternative-energy-based syntheses and processes as well as in the interaction of various process and equipment design parameters that determine performance.

New reactor and process design address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Buildings and industrial facilities in energy transition' (5.4), 'Energy storage' (5.9), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) mainly by:

- **Contributing to low-carbon economy** by enabling the introduction of renewable energy in chemical processes through electrification;
- **Improved energy efficiency in the chemical industry**, through localised heating and energy input to chemical reactions;
- **Enabling the valorisation of alternative carbon feedstock** such as biomass, CO_2 and waste contributing to **circular economy**.

Horizontal challenges:

- Reactor design and reaction engineering to fit specific requirements of non-conventional energy sources, maximising process efficiency;
- Process optimisation and integration of non-conventional energy sources into continuous chemical processes;
- Integration of non-conventional energy systems with renewable-energy electricity sources;
- Improved scalability of industrial design.

SUSCHEM PILLARS – MULTI-KETS:

The utilisation of alternative energy forms can have impact on Advanced Materials (Chapter 2) production especially from alternative feedstock.

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable the implementation and scale-up of alternative energy forms- based processes, in particular 'Laboratory 4.0 - Digital R&D' (4.1), 'Design of reactors' (4.1.3), 'Process Analytical Technologies (PAT)' 4.2, 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3 and 'Predictive maintenance' 4.5.

Alternative energy forms are expected to impact other **Advanced Process Technologies (Chapter 3)** and especially on processes related with the integration of alternative feedstock (CO_2, biomass, waste) and renewable energy: 'New reactor design and equipment' (3.1) and 'Waste valorisation process technologies' 3.11.

RD&I Actions

3.4.1 Plasma

Context: The integration of plasma-based technologies allows the utilisation of electricity as an external energy form in process industries. It also enables the application of renewable electric power into the chemical value chain. Plasma as an ionised gas with free electric charges, namely electrons and ions, offers major features:

- Temperature and energy density in plasma can significantly exceed conventional operating windows;
- Concentrations of energetic and chemically active species (electrons, ions, radicals, excited states) can be very high in a plasma;
- Plasma systems can be far away from thermodynamic equilibrium providing the extremely high concentrations of active species at simultaneous bulk temperature as low as room temperature.

Potential fields of application are the intensification of chemical reactions, CO_2 valorisation through plasma-catalytic processes, plasma gasification of waste to syngas as sustainable platform technology, all allowing the integration of renewable energy.

Specific challenges:

- Intensification of chemical reactions by plasma effects (energy density and active species, electrical conduction, internal interaction, response to electromagnetic fields);
- Heterogeneous catalyst and surface interactions/ reactions in plasma-catalytic processes for instance for CO_2 valorisation (CO_2 splitting, dry methane reforming);
- Plasma gasification: sustainable feedstock (municipal, agricultural, plastic wastes) valorisation and flexibility through process tolerance, sustainable routes to bulk and specialty chemicals;
- Industrial design and easy-scalable plasma systems (plasma type, control systems and operation, materials development, retrofit of conventional plants).

Specific expected impact: Plasma can intensify chemical processes, increase process efficiency and stimulate chemical reactions impossible in conventional chemistry. Main application areas include bulk chemistry, specialty chemistry, energy intensive industries, waste and recycling sectors with contribution to: a) development of a more circular economy through the implementation of plasma gasification to chemical recycling and waste utilisation, as well as the utilisation of CO_2 as feedstock; b) greenhouse gas emissions reduction through the integration of renewable electricity in the process industry via plasma and the chemical valorisation of CO_2; and c) increased resource and energy efficiency through the intensification of chemical processes (novel process windows, lower temperatures).

IMPACT EXAMPLES:

Example 1: The reaction intensification of plasma has been reported in CO_2 conversion into methane. A catalysed reaction was carried out at low temperature (90 °C). CO_2 conversions of 80 % and 100 % selectivity towards methane was reported in the presence of plasma, which could only be reached at 300 °C without plasma.[133]

Example 2: Plasma gasification can allow the utilisation of, for example, complex industrial fermenter by-products, which are usually hard to crack in conventional gasification. Carbon conversion efficiencies up to 89 % and near equilibrium syngas composition was reached in a microwave plasma reactor.[134]

TRL(now) & TRL(2030): Plasma gasification is already at high TRL (TRL 7-8), while other plasma technologies are currently at TRL 5-7 and are expected to be at TRL 8-9 by 2030.

3.4.2 Ultrasound

Context: Ultrasound is a mechanical sound wave with a frequency above 20 kHz and up to several GHz. Research on acoustic energy effects in chemical processing has a long history and ultrasonic devices have already found a number of commercial applications, e.g., in cleaning and decontamination or for dye dispersion and fixation in the textile industry. At 100s to 1000s of Watts it is exploited as "power ultrasound" for sonochemical applications, with frequency typically between 20 kHz and 10 MHz. Power ultrasound induces acoustic streaming and cavitation, which can be used to intensify transfer of mass, heat and momentum, and to activate chemical reactions. The chemical effects of ultrasound (radical formation) are applied in organic synthesis and degradation reactions. Mechanical effects are beneficial for leaching, extraction, crystallisation and acoustophoretic separation. However, the record of investigated processes is limited.

Specific challenges:

- Ultrasound probes are not tailored to chemical reactors, transfer of ultrasound to reactor has not yet been optimised;
- Reaction mechanisms not well understood, leading to underdeveloped models;
- Scale up.

Specific expected impact: The use of ultrasound in chemical processes enables non-contact mixing and mass transfer as well as chemical activation, which is particularly interesting for small-volume equipment such as in continuous flow systems. As such, it can be an enabler to integrate renewable electricity in chemical processes.

IMPACT EXAMPLES:

Example 1: A biorefinery concept for the complete valorisation of lignocellulosic biomass that includes a mechanical pre-treatment of the substrate with the aid of ultrasound to overcome its recalcitrance and disrupt inhibitors.[135]

TRL(now) & TRL(2030): For most of the applications there are examples to be found up to TRL 3-4. Some examples of TRL 5 are available for ultrasound-assisted (catalytic) synthesis. A number of ongoing projects are expected to raise TRL to 6 in the near future. Further investments should bring these applications in 2030 to TRL 7-9. However, there is a large number of processes that have not or scarcely been investigated yet (TRL ≤2).

3.4.3 Microwave

Context: Microwaves have been demonstrated to catalyse effectively chemical reactions mainly due to rapid, selective and volumetric heating principles. Microwaves can be used for example for the conversion of biomass and by-products: pyrolysis, carbonisation, bioactive compound extraction, and hydrolysis are just a few examples of valorisation of biomass assisted with microwaves.[136] Further, a broad range of (reactive) separation processes such as (reactive) extraction, distillation and crystallisation, but also desorption, pervaporation, demulsification and demetallisation can by intensified by the use of microwaves. Evaporative crystallisation for example can be enhanced by the use of microwave[137] irradiation that significantly speeds up solvent evaporation, resulting in rapid crystallisation and reduced particle size. Moreover, for chemical reactions, specific catalysts and especially those based on carbon or metal nanoparticles can further enhance absorption of microwaves. Finally, reactive extrusion of highly viscous materials can also be assisted by the use of microwaves that can induce efficient heating overcoming the inherent low conductivity of these materials.

Specific challenges:

- The relative contribution of thermal and non-thermal effects of microwave irradiation in a range of processes is still not well understood. Here non-thermal effects should be understood as the effect of microwaves on liquid-solid interfacial mass transfer at micro- or macroscale, or charge transport (electrons or ions) on solid surfaces, solid matrices and ionic media;
- Reactor design to maximise the potential of microwave assisted chemical reactions. Parameters such as type of reactor (batch or flow), mode (mono- or multi-), size, materials, microwave frequency, homogeneity, and penetration depth (shape) should be considered, and in many cases, these are interconnected;
- Reactor design for heat transfer related issues. When using microwave reactors, heat is mainly generated by friction and collisions between molecular dipoles. However, there are also secondary thermal phenomena, such as conduction, convection or radiation that must be considered. In the case of microwave-absorbing catalysts (such as carbonic or metal nanoparticles), heat can build-up, causing overheating or hotspots that may have a negative effect on the process, and are difficult to transfer into the bulk of the reaction mixture;
- Microwave assisted reactors need to be optimised to fit targeted reaction requirements, delivering the required amount of energy at the required rate to the required place, and in a continuous flow mode;
- Microwave-absorbing catalysts must be tailored to allow for high activity and heating rates while avoiding overheating and hotspots;
- Integration and combination of microwave with other technologies such as ultrasound or plasma must be further developed;
- Generic scale up rules for microwave assisted multiphase reactors need to be established.

Specific expected impact: The use of microwaves in chemical processes enables non-contact heating as well as reaction activation, which is beneficial for many microwave-assisted chemical reactions. It can also be seen as an enabler to integrate renewable electricity in chemical processes.

IMPACT EXAMPLES:

Example 1: Use of microwaves as part of a process intensification approach for the catalysed alkaline hydrolysis depolymerisation reaction of polyethylene terephthalate, which is currently economically unfeasible, with a potential for significant reduction of PET waste.[138]

Example 2: Microwave is considered as an option to develop innovative process for the valorisation of methane feedstock to higher hydrocarbons and liquid fuels to reduce energy consumption and CO_2 emissions.[139]

TRL(now) & TRL(2030): For most of the applications of microwave-assisted heating and catalysis there are examples to be found up to TRL 5-6. Further investments should bring these applications in 2030 to TRL 7-9.

3.5 Electrochemical, Electrocatalytic and Photo-electrocatalytic Processes

Context: Electrochemistry can provide 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 catalysis recovery are promising applications of electrochemical processes. Electrocatalysis is a subclass of heterogeneous catalysis that aims to increase the rates of an electrochemical reaction taking place at the surface of electrodes, while electro-photocatalysis enables the direct utilisation of sunlight.

Market, overall expected impact: Novel process technologies for electrochemical processes can provide new production routes for various chemicals, including through the valorisation of alternative feedstock, especially CO_2. As they also offer opportunities for direct utilisation of renewable energy in chemical processes, their contribution to reduce the environmental of chemical processes is high. In addition, electrochemical processes can provide options for storage of renewable electricity. Electrochemical processes can also contribute to a more circular economy through separation of metals in waste streams, as well as catalyst recovery.

Electrochemical, electrocatalytic and photo-electrocatalytic processes address several **Horizon Europe (HEU) clusters and areas of intervention**: 'Emerging enabling technologies' 4.3, 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Energy grids' 5.3, 'Buildings and industrial facilities in energy transition' (5.4), 'Energy storage' (5.9), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) mainly by:

- **Contributing to the development of a low-carbon economy** by enabling the introduction of renewable energy in the chemical industry through direct electrification of chemical processes;
- Enabling the **valorisation of alternative carbon feedstock**, in particular **CO_2** contributing to a more **circular economy**;
- **Sustainable management of critical raw materials** through recovery processes.

Horizontal challenges:

- Process optimisation of processes, in particular catalyst design and optimisation (see Enabling CO_2 valorisation via catalysis (3.9));
- Reactor design and engineering to achieve improved reaction control and address specific requirements of the feedstock and energy source.

SUSCHEM PILLARS – MULTI-KETS:

Electrochemical processes can have impact on **Advanced Materials (Chapter 2)** production especially for the production of polymers from CO_2-derived building blocks.

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable the implementation electrochemical processes, in particular 'Laboratory 4.0 - Digital R&D' (4.1), 'Design of reactors' (4.1.3), 'Process Analytical Technologies (PAT)' 4.2, 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3, 'Predictive maintenance' 4.5 and 'Coordination and management of connected processes at different levels' 4.8.

Electrochemical processes can benefit from other **Advanced Process Technologies (Chapter 3)** 'New reactor design and equipment' (3.1), 'Catalysis (3.9)' and 'Industrial Biotechnology' 3.10, and will impact 'Power-to-chemicals' (3.8) and 'Hydrogen production with low carbon footprint' (3.7), 'Waste valorisation process technologies' 3.11 and 'Process technologies for advanced water management' 3.12.

RD&I Actions

3.5.1 Electrochemical reactors and processes

Context: Current applications for electrochemical production of chemicals is still limited to a few and long-established electrolysis processes like Chlor-Alkali electrolysis. Electrolysis processes especially for bulk chemicals production can significantly contribute to the reduction of the GHG emissions by using climate-neutral electricity to produce value-added products and especially when alternative carbon feedstock (including CO_2) is converted. Efforts to broaden the production scope of electrolysis processes are enhanced. Strong focus is given to the electrochemical

CO_2 reduction delivering gas mixtures ($CO+H_2$), C2 compounds like ethylene and acetate or even C4-C6 chemicals by subsequent fermentation processes. Electrochemical conversion is not restricted to CO_2 and thus enables sustainable production of a broader spectrum of chemical products, e.g. lignin types and sugars like glucose were tested as feedstock to produce electrochemically value-added. Electrochemical processes also offer options for storage of renewable electricity through Power-to-X technologies (see **3.7** and **3.8**).

Specific challenges:

- The electron transfer at the electrode–electrolyte interface is mostly considered to be the decisive factor for electro-conversion. Electro-catalysts are crucial for synthetic conversion;
- Owing to the stability and lifetime of many organic radicals, there is a second regime that needs to be controlled in case of electro-organic synthesis applications to achieve the desired transformation. 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);
- Advanced concepts in electro-organic synthesis focus on flow processes, allowing simplified upscaling and minimising need for a supporting electrolyte. Innovative electrolyte and electrode systems have to be elaborated to enable novel transformations. Thus, actual limits resulting from current electrode materials will be circumvented.

Specific expected impact: Electrochemical reactors and processes as alternative to conventional process technologies to achieve a significant impact on reducing GHG emissions. In fine chemical and pharmaceuticals synthesis, i.e. organic-electro-synthesis, the impact can be even more due to the unique reactivity of electro-catalytic reactions. As only electrons serve as reagents, the generation of reagent waste is efficiently avoided. Moreover, stoichiometric reagents can be regenerated and allow a transformation to be conducted in an electro-catalytic fashion. This gives rise to inherently safe processes, reduces the number of steps of many syntheses, allows for milder reaction conditions and provides alternative routes to access desired structural entities.

IMPACT EXAMPLES:

Example 1: Development of a combined electrochemical technology for the simultaneous conversion of CO_2 to ethylene at the cathode, water oxidation to hydrogen peroxide at the anode and a subsequent chemical conversion of both intermediates to ethylene oxide and oligo-/polyethylene glycol in a cascade.[140]

Example 2: Development of an integrated process for the production of high-value C2 chemicals from carbon dioxide using electrochemistry, moving the technology to TRL 6.[141]

TRL(now) & TRL(2030): The TRL of electrochemical methods as alternative to conventional process technologies (e.g. for CO_2) and including electrolytes such as ionic liquids/non-aqueous electrolytes is at TRL 4-5. More R&I on demonstration activities at TRL 6-8 needs to be considered by 2030.

3.5.2 Electrochemical processes for recovering valuable materials, including catalyst

Context: Electrochemical processes can offer sustainable options to recover valuable materials from waste since no additional oxidising or reducing chemicals are needed. The reactive components in electrochemical processes are electrons. Chemical selectivity of electrons can be tuned by application of the appropriate potential. The chemical kinetics can be controlled by adjusting the current density. For a minimal carbon footprint, the electrical energy used should be generated by a renewable power sources, e.g. wind turbines or photovoltaic systems.

There are several electrochemical methods to recover metal ions or remove organic molecules from industrial wastewater or urban sewage. Examples are removal of toxic heavy metals and recovery of high value catalysts, e.g. platinum. Even recycling of low value salts, e.g. sodium chloride, can become a cost factor in times of zero liquid discharge. Alternative solvents such as ionic liquids, having a large electrochemical window, have been extensively studied as promising media for electrochemical processes and electrodeposition. Selectivity of electrochemical processes results from applying a defined electrode potential. This can be used to remove a metal ion from a mixture of different ions.

The polarisation of carbon-based electrode material can be used in an electrochemical adsorption/desorption process, to transfer organic molecules or ions from one solution into another one. The removal of organic molecules - mostly in

low concentration is necessary to protect electrochemical components from becoming passivated.

Specific challenges:

- Corrosion-resistant and inexpensive electrode materials for efficient processes;
- Carbon-based materials suitable for an efficient electrosorption;
- Minimisation of side products from electrolysis and identification of critical side products;
- Limitation of calcification of electrodes;
- Optimised design of electrochemical cells and robust media;
- Development of sensors for chemical oxygen demand;
- Design of efficient scale-up.

Specific expected impact: Electrochemical processes for waste treatment to achieve a significant impact in recovering valuable materials (e.g. metals, critical raw materials), thus minimising waste, and reducing CO_2 emissions. This contributes to foster efficient use and recycling of critical raw materials, and therefore to the new Circular Economy action plan.

IMPACT EXAMPLES:

Example 1: A first of a kind economically and environmentally viable mobile commercial metallurgical system based on advanced hydrometallurgical and electrochemical technologies able to produce cobalt metal from black mass containing cobalt from different sources of waste streams such as spent batteries and catalysts.[142]

TRL(now) & TRL(2030): The TRL of electrochemical methods depends on the corresponding technique. In most cases, electrochemical processes for water or waste treatment is at TRL (3- 5). More R&I on demonstration activities at TRL 5-7 needs to be considered by 2030.

3.5.3 Photo electrochemical reactors

Context: Photo electrochemical processes utilise light, usually sunlight, to power an electrochemical reaction and represent an integrated approach versus using photovoltaics with coupled electrolysers. The integration promises higher efficiency and lower costs as less conversion steps and components are required. The use of this technology is explored both for the generation of hydrogen via water splitting and for carbon-based chemicals and fuels from CO_2 reduction (solar fuels). The implementation of these photo-electrochemical processes, from very small laboratory cells (with photoelectrodes of around 1 cm^2), into devices requires efficient and scalable reactor concepts that are inexpensive and can be easily mass-produced. These devices need to consider the optimal collection of sunlight at the photoelectrode(s) surface, minimise resistive losses and ensure an efficient collection and separation of the products.

Specific challenges:

- Improved efficiency of photo electrochemical processes which are scaled-up to around 50 cm^2 has been attempted, however dramatic losses of efficiency were observed, revealing significant demand for further research in this area;[143,144]
- Improved designs for reducing resistive losses within both the photoelectrode(s) and the electrolyte as well as better separation and collection of the products;
- More research on manufacturing techniques for stable, efficient and homogeneous large surface area photoelectrodes. Cell designs should ideally use abundant, inexpensive materials and use manufacturing techniques which enable facile mass-production.

Specific expected impact: Projections for photo electrochemical technologies are difficult due to their low TRL. However, such technologies would represent a real breakthrough, as they would enable the utilisation of CO_2 as an alternative carbon source, independent from the availability of renewable electricity. The technology will also benefit from improvement in efficiency from the photovoltaics industry.

IMPACT EXAMPLES:

Example 1: Cost-effective, solar-driven H_2 production by introducing an anion-exchange polymer membrane and porous hydrophobic backing layer in a tandem photo electrochemical cell, achieving a photo-electrolysis device with solar to-hydrogen efficiency of 10 % and a prospective lifetime of 20 years.[145]

Example 2: Design and optimisation of a photo-electro-catalytic (PEC) cell prototype for the production of fuels and chemicals using CO_2, water and solar energy aiming at 10 % efficiency, using ultra-thin layers and nanoparticles of metal or metal oxide catalysts for both half-cell reactions.[146]

TRL(now) & TRL(2030): Photo-electrochemical reactors are currently at TRL 2-4. More demonstration activities on exploring new designs to achieve at least TRL 5-7 by 2030 need to be undertaken.

3.6 Power-to-Heat

Context: Providing heat to drive chemical processes contributes significantly to the total energy demand of the chemical sector. Today's production of industrial heat relies mostly on fossil fuels, either using boilers for steam production or furnaces, and thus it is responsible for a large portion of the CO_2 emissions.[147] Electrical heating technologies (Power-to-Heat) create the opportunity to reduce CO_2 emissions, when the electricity is produced from renewable sources such as wind, solar or hydropower.

Market, overall expected impact: The European vision of a sustainable, low-carbon and climate friendly economy requires a paradigm change for the chemical industry supported by technological breakthroughs such as power-to-heat.

Power-to-Heat address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Energy grids' 5.3, 'Buildings and industrial facilities in energy transition' (5.4), 'Energy storage' (5.9) and 'Circular systems' (6.7) mainly by:

- **Contributing to the development of a low-carbon economy** by enabling the indirect introduction of renewable energy in the chemical industry through the utilisation of electricity to produce heat and steam;
- **Significant CO_2 emissions reduction** since heat is responsible for most of the CO_2 emissions in the chemical sector.

Horizontal challenges:

- Energy efficiency of electricity-based heating systems for low and high temperature heat;
- Integration of novel heating systems with renewable energy electricity sources;
- Materials for high temperature heating.

SUSCHEM PILLARS – MULTI-KETS:

There is a horizontal dimension of Enabling Digital Technologies (**Chapter 4**) to enable the implementation of Power-to-Heat, in particular 'Laboratory 4.0 - Digital R&D' (4.1), 'Process Analytical Technologies (PAT)' 4.2, 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3, 'Advanced data analytics and artificial intelligence' 4.4 and 'Predictive maintenance' 4.5.

Power-to-Heat can benefit from other Advanced Process Technologies (**Chapter 3**) in particular 'New reactor design and equipment' (3.1) and 'New reactor and process design using non-conventional energy forms' (3.4).

RD&I Actions

3.6.1 Electrical heat pump technologies

Context: A heat pump can upgrade a source of waste heat to a higher temperature level needed to drive a process. Heat pump applications provide solutions for recovery and re-use of low-grade heat sources and upgrade this heat towards the temperature level needed to drive a process. This creates a circular use of heat, reducing the need for cooling towers, and reducing thermal loads on the environment. Major technology options are:

- **Steam compression technology (mechanical vapour recompression)** allows to recover heat from low grade steam and hot condensate and upgrade this to higher pressure and temperature for re-use in processes. The specific strength of this technology is the ease to integrate such a compression system in the existing steam system of a process or site. This matches to a broad range of applications throughout various processes, as steam is the dominant heating utility in the process industry;

- **Closed cycle compression heat pumps:** current commercially available Industrial heat pump systems are able to provide heat at a temperature of 90 °C. New developments in heat pump technology aims to increase the temperature level for heat delivery towards 150 °C, allowing to provide low pressure steam. The objective would be to develop heat pump technologies providing a temperature level above 200 °C with processes less energy intensive than steam compression.

Specific challenges:

- **Cost reduction of heat pump systems** to improve competitiveness against fossil-based heating systems;
- **Increased temperature for heat delivery**, developing new working fluids for advanced heat pump cycles, i.e. sorption and thermoacoustic and hybrid cycles;
- **Development of compressor technologies** for high temperature heat pumps;
- **Development of smart process integration of heat pumps**, with heat pump cycles integrated in specific processes, using waste heat from the process to provide process heat;
- **Development of steam compression technologies** for integration in steam-utility systems.

Specific expected impact: The implementation of industrial heat pump technology contributes to the CO_2 emission reduction targets. For example, the impact of the implementation of steam recompression in the production of six major chemical building blocks by 2050 has been estimated at 2.2 million t CO_2 emissions reduction per year.[148]

TRL(now) & TRL(2030): For heat delivery at temperatures up to 120 °C the technologies are at TRL 7. More research is needed for temperature heat pump technologies operating at 200 °C and above to bring these from TRL 3-5 to demonstration level by 2030.

3.6.2 Electrical heating technologies (utility level)

Context: Electrical heating at the utility level of a process can replace gas/oil fired heating systems by electrical heating systems. The primary processes are not directly changed by such a modification. Examples are electric boiler systems and electric furnaces and ovens. The implementation of electrical heating systems will require large amount of climate-neutral electricity. Major priorities are:

- **Electric steam production.** Electric boilers are already available commercially, but operational costs are high. The combination with steam recompression systems should be considered;
- **Electric ovens and furnaces.** In the chemical industry the steam cracking of naphtha and steam methane reforming process are examples of the use of gas fired furnaces. Replacing the gas fired heating of these furnaces by electric heating (E-cracker) is a feasible alternative that does not directly interfere or change the reforming process;
- **Hybrid heating systems**, switching between electrical heating and gas fired heating, as demand response to provide flexibility to the electricity grid, and without changing the quality or quantity of heat being produced, neither interfering with the core process. The implementation of industrial hybrid heating solutions provides a large potential (MW scale) of flex-capacity, that supports the further growth of variable renewable electricity.

Specific challenges:

- **Reduction of high operational costs** to improve cost competitiveness compared with current gas/oil fired heating systems;
- **Upscaling of electric oven and furnaces, and hybrid heating systems**, necessary to cope with the requirements of large utility capacities;
- **Integration of systems**, to work in combination with renewable energy-based sources and heat recovery systems.

Specific expected impact: For example, the impact of the implementation of electricity-based steam in the production of six major chemical building blocks by 2050 has been estimated at 20 million t CO_2 emissions reduction per year.[149]

TRL(now)&TRL(2030): Electric steam systems with steam recompression and hybrid heating systems, currently at TRL 6-7, should be implemented by 2030. As for electric ovens and furnaces for cracking and reforming application needs to be moved from current TRL 3-5 to a TRL 7-8 by 2030.

3.6.3 Electrical heating technologies (process level)

Context: Electrical heating at the process level refers to changes in the type of heating applied to a process that requires a redesign of the specific heating step. An example of such an application is the change from drying of a product by hot air to drying by means of microwave heating. Applications for these types of Power-to-Heat conversions are very process and/or product specific, and in general require a significant modification in one or more process steps.

Major options can be:

- **Di-electric heating.** Microwave heating and radio-frequency heating can provide specific advantages compared to traditional heating methods, leading to improved process control, higher throughputs or improved product quality;
- **Infrared heating.** Electric infrared (IR) is very effective in applications where only the surface of an object needs to be heated. Rapid IR heating offers the opportunity to provide a faster, cheaper and less energy intensive alternative to traditional gas-fired convection ovens;
- **Induction heating.** Electromagnetic induction heating utilises a changing magnetic field, to induce electrical eddy currents in the target material to induce heating of the material. Induction systems are sometimes used in applications where only small selected parts need to be heated but is mostly used as a melting technique for non-ferrous alloys.

Specific challenges:

- **Reduction of high operational costs** to improve competitiveness compared with current gas/oil fired heating systems;
- **Upscaling of electric oven and furnaces, and hybrid heating systems**, necessary to cope with the requirements of large capacities in industrial environments.

Specific expected impact: High temperature heat accounts for a significant part of the CO_2 emissions from the chemical sector. Electrification technologies for e-crackers would therefore be a real breakthrough with high potential on reducing GHG emissions of the chemical sector (including chemical recycling processes).

IMPACT EXAMPLES:

Example 1: Development of renewable electricity-driven steam crackers (850 °C) to break down naphtha into olefins and aromatics for further processing, has the potential of cutting down CO_2 emissions by as much as 90 %. Metallic materials that can withstand the high electrical currents and high temperatures in the reactor will be necessary. [150]

TRL(now)&TRL(2030): Electric ovens and furnaces for cracking and reforming application needs to be moved from current TRL 3-5 to TRL 7-8 by 2030 including materials developments.

3.7 Hydrogen Production with Low-carbon Footprint

Context: In the EU, it is estimated that 325 TWh[151] of hydrogen is used as feedstock every year, mostly in the refining and chemical industries, mainly for ammonia and methanol production.
Some 55 % of the hydrogen produced around the world is used for the manufacture of ammonia (mainly for fertilisers), 25 % for the processing of fossil fuels in refineries and 10 % for the production of methanol (for the production of polymers). Currently the production of hydrogen is responsible for 830 million tons of CO_2 emissions per year at a global scale[152] mainly caused by the highly energy consuming process of Steam Methane Reforming (SMR). The development of hydrogen production routes with a low-carbon footprint is therefore of high interest. The technologies already developed to produce sustainable low-carbon footprint hydrogen are based on water electrolysis[153], which currently accounts for about 5 % of the hydrogen worldwide produced. The main electrolysis technologies are alkaline water electrolysis (AWE), polymer electrolyte membrane water electrolysis (PEM) and solid oxide electrolysis (SOE). Other technologies of interest are methane pyrolysis and water photolysis (covered under 'Photo-electrochemical reactors (3.5.3)').

Market, overall expected impact: The production and utilisation of hydrogen with a low-carbon footprint can contribute to a significant reduction of CO_2 emissions from the chemical sector. In addition, such technologies can be used for energy storage applications (balancing electricity supply and demand), or as alternative fuel in the transport sector.

Technologies for the production of low-carbon hydrogen address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Emerging enabling technologies' 4.3, 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Energy grids' 5.3, 'Buildings and industrial facilities in energy transition' (5.4), 'Clean, safe and accessible transport and mobility' (5.7), 'Energy storage' (5.9) and 'Circular Systems' (6.7) mainly by:

- **Contributing to the development of a low-carbon economy** by production and utilisation of low-carbon hydrogen in the chemical industry and other sectors. In addition to enabling the introduction of renewable energy in the industry, water electrolysis technologies can provide options for renewable electricity storage;
- Enabling the **valorisation of alternative carbon feedstock** to produce chemical building blocks and fuels, in particular from **CO_2**, contributing to a more **circular economy**.

Horizontal challenges:

- Further scale up of the existing technologies (e.g. alkaline, PEM);
- Improve electrical efficiencies of the electrolysers technologies;
- Robustness of processes for low-carbon hydrogen production;
- Disruptive technologies to enable large-scale production of hydrogen with a low-carbon footprint independently of renewable electricity availability.

SUSCHEM PILLARS – MULTI-KETS:

Advanced Materials (Chapter 2) can have an impact on the production of hydrogen with a low-carbon footprint through innovation in 'Membranes for gas separation' (2.7.2).

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable the production of hydrogen with a low-carbon footprint in particular 'Design of reactors' (4.1.3), 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3, 'Predictive maintenance' 4.5 and 'Coordination and management of connected processes at different levels' 4.8.

Hydrogen production processes can benefit from other **Advanced Process Technologies (Chapter 3)** in particular 'New reactor design and equipment' (3.1), 'Power-to-Heat' (3.6) and 'Catalysis' (3.9) and will impact 'Power-to-chemicals' (3.8' and 'Industrial Biotechnology' 3.10. The direct utilisation of sunlight to produce hydrogen via water photolysis is covered under 'Photo electrochemical reactors' (3.5.3).

RD&I Actions

3.7.1 Alkaline water electrolysis (AWE)

Context: Alkaline water electrolysis is a mature technology and the most common and installed electrolysis system. The alkaline electrolysis cells use nickel catalysts at both electrodes, electrolyte solutions and inexpensive meshes as contact elements. The strength of alkaline water electrolysis is its commercial availability due to its high technology readiness level at large scale (MW range). As a consequence several high capacity AWE-electrolysers are operational worldwide. The investment costs are relatively low. Finally, AWE hydrogen is of high purity. To couple AWE to renewable energy sources in a sustainable fuels and chemicals scenario, several challenges must be overcome.[154,155,156]

Specific challenges:

- Reduction of ohmic losses;
- Improvement of gas crossover for higher pressure operations;
- Increasing the flexibility of the AWE process (i.e. reduce the start-up and shutdown ramps) towards a more dynamic operation;
- Demonstration of multi-MW scale alkaline electrolysers with reduced footprint and greater ease of commissioning and operation is required.[157]

Specific expected impact: The demand for low carbon hydrogen in 2030 will be very high and more flexible and efficient AWE will contribute to the transition of the energy system towards a sustainable future.

TRL(now) & TRL(2030): Alkaline electrolysers are a mature technology in the MW range for industrial use and require incremental innovation to adapt to new markets requirements, the expected electrolyser capacity on the market in 2030 will be > 100 MW.

3.7.2 Polymer electrolyte membrane water electrolysis (PEM)

Context: PEM electrolysers have high investment costs (noble metals, membranes), especially in comparison to alkaline electrolysis, and PEM electrolysis requires high water purity. It is currently a highly competitive approach for splitting water to generate hydrogen. PEM electrolysis cells use a thin polymeric electrolyte membrane. At the cathode usually, a platinum catalyst is used for the hydrogen evolution, whereas at the anode an iridium catalyst is deployed for the oxygen evolution. Its advantages are high power density and cell efficiency, provision of highly compressed and pure hydrogen, and flexible operation. PEM electrolysers have a very fast response time. It is a reliable technology with simple and compact design. The modular design allows a significant cost reduction potential.

Key specific challenges:

- Reducing iridium in PEM anodes (limiting the growth of PEM technology);
- Research on new alternative catalysts;
- Optimising electrolysis peripheral components (beside electrodes), such es anion exchange membranes, porous transport layers, bipolar plates, etc;
- Reducing the system capital, hydrogen and stack costs.

Specific expected impact: Due to its flexibility and dynamic operation mode PEM electrolysis is expected to be a key enabler for Power-to-X applications and thus also the European energy transition.

TRL(now) & TRL(2030): PEM electrolysers are commercially available, and a very dynamic market development is currently being observed and several manufacturers are already offering modules in the MW range. For specific applications, the TRL level is between 5 and 8. Towards 2030, an important scale-up will take place with PEM electrolysers with higher capacity.

3.7.3 Solid oxide electrolysis (SOE)

Context: Solid oxide electrolysis cells (SOEC) use oxidic membranes coated with different catalysts to split water and they operate at high temperatures (500-850 °C). The ceramic electrolyte conducts oxygen anions from the cathode (hydrogen generation) to the anode where oxygen is generated. The SOE technology has the highest electrolysis efficiency and has the advantage of low capital costs. The high temperature level allows for heat integration with other (up- and downstream) processes. Another example is the potential use for co-electrolysis of both steam and CO_2, producing syngas, from which hydrocarbons such as liquid fuels can be produced. In addition to the fundamental efficiency advantages, the reversibility of the process

offers another important advantage: an SOE-based cell can be simultaneously used as a fuel cell or as an electrolysis cell.

Specific challenges:

- Increase the scale-up potential;
- Reduction of mechanical stress on solid oxide material as current SOE based cells have a limited lifetime because of high operating temperature and the resulting affected material stability;
- Increase the flexibility which is limited owing to the need for constant loads.

Specific expected impact: Although currently the technology is not able to significantly contribute to hydrogen production, SOE has the potential to be cost-effective, environmentally friendly, and highly efficient. The future impact of SOE depends on overcoming the main challenges of SOEC, especially scale-up.

TRL(now) & TRL(2030): The technology readiness level is lower than other low temperature electrolysis technologies (TRL 5). First small units are available, and SOE cells should reach TRL level 7-8 by 2030.

3.7.4 Methane pyrolysis

Context: Methane pyrolysis is a thermal non-catalytic pyrolysis process, splitting methane by using a high temperature reactor. Current results of R&D activities prove that the hydrogen production by methane pyrolysis, with a conversion rate of up to 78 % at temperatures of around 1200 °C, is possible. The carbon by-product (elemental solid carbon) can subsequently be used to produce steel or aluminium, lightweight construction materials or in battery production.[158] The pyrolysis of methane enables hydrogen production without direct CO_2 emissions at low energy consumption (thermodynamic minimum effort). Based on the thermodynamics the energy demand of methane pyrolysis is 87 % lower compared to water electrolysis.

Key specific challenges

- New reactor design with adapted heating system and materials;
- Economic viability which will be impacted by various parameters including the value of the by-products.

Specific expected impact: The demand of electricity for methane pyrolysis is much lower than for water electrolysis technologies. This technology therefore presents an opportunity for large scale production of hydrogen with a low-carbon footprint, in the context of limited availability of climate neutral electricity which can be a major limitation for water electrolysis technologies.

IMPACT EXAMPLES:

Example 1: The concept of producing hydrogen from natural gas, avoiding the release of CO_2 by using molten metal as the liquid medium in a bubble column reactor has been proven. Key technological aspects have been tested to develop an industrial scale process.[159,160]

TRL(now) & TRL(2030): The methane pyrolysis technology has currently been successfully demonstrated at TRL 3-5. A large-scale demonstration plant of this new process is expected by 2030.

3.8 Power-to-chemicals

Context: Power-to-X processes use electricity from renewable energy sources, to convert water and CO_2 into carbon-containing chemical building blocks (e.g. methanol). Such technologies can contribute to carbon circularity and reduce CO_2 emissions. Power-to-X technologies can also be applied to the production of ammonia. Power-to-X process technologies can also provide options for renewable electricity storage, contributing to grid stability via the production of energy carriers (e.g. methane, methanol, ammonia).

Market, overall expected impact: Through the production of syngas or large volume chemical building blocks such as methanol, power-to-chemicals technologies can play a key role in the introduction of renewable electricity in the chemical industry and they have the potential to decrease significantly the emissions from the sector.[161]

Power-to-chemicals technologies address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Emerging enabling technologies' 4.3, 'Circular industries' 4.8, 'Low-carbon and Clean Industries' 4.9, 'Energy supply' 5.2, 'Energy grids' 5.3, 'Buildings and industrial facilities in energy transition' (5.4), 'Clean, safe and accessible transport and mobility' (5.7), 'Energy storage' (5.9) and 'Circular Systems' (6.7) mainly by:

- **Contributing to the development of a low-carbon economy** by enabling the introduction of renewable energy in the chemical industry and providing options for renewable energy storage;
- Enabling the **valorisation of CO2 as alternative carbon feedstock** contributing to a more **circular economy**.

Horizontal challenges:

- Performance improvements beyond energy efficiency, to improve process metrics;
- Catalyst design (see 'Enabling CO_2 valorisation via catalysis' (**3.9.3**));
- Reactor design and engineering to achieve improved reaction control;
- Further scale up of the technologies developed;
- Higher production cost than fossil-based route due to high OPEX.

SUSCHEM PILLARS – MULTI-KETS:

Advanced Materials (Chapter 2) can have an impact on power-to-chemicals through innovation in 'Membranes for gas separation' (2.7.2).

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable Power-to-chemicals in particular 'Design of reactors' (4.1.3), 'Cognitive plants: (real-time) process simulation, monitoring control and optimisation' 4.3, 'Predictive maintenance' 4.5 and 'Coordination and management of connected processes at different levels' 4.8.

'Power-to-chemicals' can benefit from other **Advanced Process Technologies (Chapter 3)** in particular 'New reactor design and equipment' (3.1), 'Hydrogen production with a low-carbon footprint' (3.7), 'Catalysis' (3.9) and 'Industrial Biotechnology' 3.10.

RD&I Actions

3.8.1 Power-to-syngas

Context: The production of syngas from water, CO_2 and renewable energy can be realised in different ways. The electrolysis of water (e.g. with SOEC (**3.7.3**)) can be coupled with the Reverse Water Gas Shift Reaction (RWGSR) where CO_2 is converted to CO with the production of water at high temperature. This causes a decrease in overall hydrogen yield, but the synthesised water can be recycled into the process. Coupling of the two processes followed by RWGSR of CO_2 is challenging in operation due to different reaction conditions. Two other production pathways for syngas, the low and high temperature co-electrolysis of water and CO_2, using electricity from renewable sources, are very powerful techniques to produce various syngas mixtures. In these processes, the chemical bonds in the water and CO_2 molecules are broken simultaneously to form hydrogen and CO. Syngas is a feedstock for various chemical processes, including the production of large-scale chemical building blocks.

Specific challenges:
See Horizontal challenges (3.8) and especially the scale-up of the technology which is currently available at only small scale.

Specific expected impact:
See Market and overall expected impact (3.8).

IMPACT EXAMPLES:

Example 1: Syngas production from CO_2 and water to produce aviation fuel via Fischer-Tropsch synthesis.[162]

Example 2: Production of syngas from water and CO_2 via electrolysis followed by conversion to alcohols (hexanol / butanol) via fermentation process.[163]

TRL(now) & TRL(2030): Power-to-syngas technologies have achieved various TRLs depending on the low-carbon hydrogen production and conversion route that depends itself on the applications. More R&I on demonstration and optimisation activities are needed to achieve a TRL 5-7 by 2030.

3.8.2 Power-to-methanol

Context: Current power-to-methanol processes use syngas produced by catalysed electrolysis of water and CO_2 to produce methanol that can be used for energy storage, synthetic fuels and base chemicals. The operation of the catalytic reaction takes place at pressures >70 bar and temperature below 250 °C. These conditions help to stabilise the catalyst but result in low conversion rates. Power-to-methanol produces high energy density products and feedstock for various chemical reactions.

Specific challenges:
See Horizontal challenges (3.8). Research should especially address catalyst development to increase its stability, selectivity and tolerance towards water.

Specific expected impact: See Market and overall expected impact (3.8). Additionally, a recent study shows the projected high impact of power-to-methanol technology with an evaluated CO_2 emissions reduction of 30.3 million t CO_2 /y in 2050 in an ambitious deployment scenario of CO_2-to-methanol and methanol-to-olefins.[164]

IMPACT EXAMPLES:

Example 1: Demonstration pilot plant able to produce 1 ton of methanol per day used for production of platform chemicals and renewable fuels by capturing more than 1.5 tons of CO_2 per day.[165]

Example 2: Production of methanol from CO_2 and water in a modular containerised system with an energy efficiency of 74 %.[166]

TRL(now) & TRL(2030): Some power-to-methanol technologies are at TRL 7-8. More R&I activities can improve the efficiency and large-scale demonstrations of first-generation technologies need to be considered by 2030.

3.8.3 Power-to-fuels

Context: Power-to-fuels processes convert syngas, produced from CO_2 and water, to synthetic fuels like kerosene or diesel via, for example, Fischer-Tropsch synthesis for applications in energy, traffic and transportation sector. The technology can provide the transport sector with fuels with a much lower carbon footprint. Synthetic fuels are highly promising as alternatives to fossil-based fuels due to their high energy density. One of the main advantages of power-to-fuels is the production of high energy density of products with long-term energy storage application, and the compatibility with the existing infrastructure for storage, transport and application.

Specific challenges:
See Horizontal challenges (3.8). Additionally, for a decentralised operation, the reactors need to be smaller and the exothermicity of the reaction needs to be better controlled. Therefore, catalysts need to be developed that operate at low temperatures with higher selectivity.

Specific expected impact: See Market and overall expected impact (3.8). Additionally, a recent study shows the projected high impact of power-to-fuels technology with an evaluated CO_2 emissions reduction of 110 million t CO_2 /y in 2050 in an ambitious deployment scenario of CO_2-to-methanol and CO_2-to-fuels technologies.[167]

IMPACT EXAMPLES:

Example 1: Demonstration of the production of synthetic fuels (such as gasoline, diesel, kerosene) from CO_2 and water with renewable electricity with an overall efficiency up to 65 %, with potential CO_2 emission reduction of 3.14 tons of CO_2 for each ton of fuel produced.[168]

TRL(now) & TRL(2030): Power-to-fuels technologies are at TRL 4-7, depending on temperature regime and considered processes, with some small scale operation units at TRL 4. More R&I on demonstration and optimisation technologies to achieve a TRL 8-9 needs to be considered by 2030.

3.8.4 Power-to-methane

Context: The power-to-methane process couples renewable hydrogen production via electrolysis (e.g. technologies mentioned in chapter 'Hydrogen production with low-carbon footprint (3.7)') with subsequent methanation of CO_2 and H_2 to methane at temperatures between 300 and 600 °C at moderate pressures. Currently, operating processes have reached the size of demonstration projects with high efficiencies of more than 75 %. Methane can be used as a chemical feedstock to produce bulk chemicals and power-to-methane can provide options for large-scale storage of renewable electricity, using existing gas grid infrastructures. Further, power-to-methane allows for decentralised production, long-term energy storage and it is compatible with existing infrastructure.

Specific challenges:
See Horizontal challenges (3.8). Specific challenges related to the application include:

- Optimisation of reactor concepts and designs to achieve operational stability and flexibility;
- The exothermicity of the process needs to be safely controlled;
- Catalyst design for low-temperature operations, with increased activity and tolerance to poisoning;
- Low tolerance to instabilities during operation.

Specific expected impact: Unlimited feed-in of methane in the existing gas grid possible, less dependence on fossil resources, closed carbon cycle, reduction of CO_2 net emissions.

IMPACT EXAMPLES:

Example 1: Achieving a conversion efficiency of > 85 % through a highly efficient Power-to-Gas (P2G) technology with methane as a chemical storage and by thermally integrating high temperature electrolysis (SOEC technology) with methanation.[169]

TRL(now) & TRL(2030): Power-to-fuels technologies are at TRL 4-7, depending on temperature regime and considered processes, with some small scale operation units at TRL 4. More R&I on demonstration and optimisation technologies to achieve a TRL 8-9 needs to be considered by 2030.

3.8.5 Power-to-ammonia

Context: Power-to-ammonia processes convert nitrogen and hydrogen to ammonia used in agriculture, food and health industries, energy storage, or large-scale chemicals. For sustainable ammonia production the reaction should take place at low pressures and temperatures. One feasible approach is the electrolytic synthesis of ammonia using renewable hydrogen from electrolysis of water. The main challenges that need to be addressed lie in the optimisation of the Ru-based catalyst for operation under dynamic changes, due to changes in the availability of renewable energy and in increasing the current density for a more efficient process. However, an increase in current density in electrochemical devices would affect the final costs of ammonia enormously and lead to more than double the price compared to methane. In case of ammonia production for the energy sector the price of ammonia is still too high. Power-to-ammonia contributes to fossil-free production of fertilisers and offers large-scale seasonal storage as well as large energy storage potential.

Specific challenges:

- Optimisation of catalyst/electrodes to meet fluctuating energy supply;
- Availability of feedstock only decentralised;
- Decentralised plant necessary;
- Low efficiency.

Specific expected impact: Power-to-ammonia to achieve a significant impact on environmentally friendly, sustainable production of fertilisers and energy supply, reduction of nitrogen input in the environment, less dependence on fossil resources, carbon-free energy based on ammonia.

IMPACT EXAMPLES:

Example 1: Demonstration pilot plant capable of producing ammonia at the rate of 20 kg per day with hydrogen produced through the electrolysis of water with power generated by solar power equipment.[170]

TRL(now) & TRL(2030): Power-to-ammonia technology is currently at TRL 5-6.

3.9 Catalysis

Context: Catalysis is an interdisciplinary and overarching technology in the process and chemical industry. The academic and industrial research on catalysis underpins several strategic sectors of the EU economy: from energy to the production of materials and other chemical products for commodities. Catalysis has a key enabling role in addressing societal and global challenges, with an expected contribution in recycling and valorisation of waste streams. As such, overall, it opens new routes to sustainable and environmentally friendly processes and products.

The current challenging endeavour is to explore a paradigm shift in better addressing innovation in catalysis at a European level. This includes a better coordination between European and national activities and the support of large-scale research infrastructures. European catalysis research needs an integrated and coordinated approach to several disciplines and stakeholders along the value-chain to be more successful. This would essentially drive the TRLs toward spanning from rather low fundamental research on catalysis up to demonstration levels. It is needed to stimulate innovation to create breakthrough sustainable solutions and to promote the development and growth of KETs.

Overall, innovation priorities should focus on the catalytic valorisation of: i) biomass feedstock, ii) waste – including plastics waste, iii) CO_2, and iv) light hydrocarbons, along with addressing horizontal challenges such as process intensification and rational catalyst design.

Market, overall expected impact:
Approximately 90 % of chemical processes use a catalyst for efficient production.[171] At a global level technical improvements in catalyst and related processes could reduce energy intensity for the top 18 energy intensive large volume chemicals by 20 % to 40 % as a whole by 2050, combining all scenarios.[172] In absolute terms, improvements could save as much as 13 EJ and 1 Gt of carbon dioxide equivalent (CO_2-eq) per year by 2050 vs. a "business-as-usual" scenario.[173] Catalysis is expected to have an essential role for the sustainable valorisation of alternative carbon feedstock through process optimisation.

Catalysis addresses several **Horizon Europe (HEU) clusters and areas of intervention:** 'Key Digital technologies' 4.2, 'Advanced Materials' 4.4, 'Circular industries' 4.8, 'Low-carbon and clean industries' 4.9, 'Energy supply' 5.2, 'Clean, safe and accessible transport and mobility' (5.7), 'Energy storage' (5.9), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7).

Horizontal priorities:
- Rational design of new catalysts, combining computational tools, combinatorial design and high-throughput screening;
- Improved catalyst characterisation techniques/ methods;
- Novel characterisation tools for in-situ monitoring of reaction and catalyst over time;
- Advanced catalyst production techniques e.g. 3D-printing to promote intensification of catalytic processes (see **3.1.9**);
- New reactor design: e.g. coated microchannel reactors, monolithic reactors, coated heat exchangers;
- Intensification of catalytic processes to develop and design more efficient processes (e.g. integration of the catalyst to the reactor structure (see **3.1**));
- Catalytic processes intensification by combining reaction and separation (e.g. by membranes);
- Catalytic processes optimisation for application of non-conventional energy forms (e.g. ultrasound or microwaves);
- New catalyst concepts and formulations with versatile applications in catalysis, including integrating new types of materials;
- Multifunctional catalysts, combination of homogeneous and heterogeneous catalysts design.

3.9.1 Enhancing biomass catalytic valorisation

Context: The production of chemicals and energy to date is mostly using fossil resources. Growing worldwide demands also leads to a higher need for more sustainable solutions and feedstock diversification. Targeted organic molecules (polymers, chemicals, fuels) could be obtained from biomass and biomass-based waste processing, with control on chemical structure and performance in downstream applications. The positive sustainability impact of such processes should be assessed, including demonstrating the economic scalability.

Process intensification and continuous processes to reduce costs and environmental impact should be realised. However, reaching a higher technology readiness level, for example on lignocellulosic biomass-based chemical processes, has been a challenge. RD&I actions should thus concentrate on more efficient conversion processes, with fewer steps resulting in competitive, low CAPEX and OPEX technologies. RD&I actions can consider chemical, physical or biotechnological solutions or sustainable combinations thereof, with catalysis having the

key role in these technology pathways. Technology priorities in this area encompass, amongst others: catalysis in biomass liquefaction, catalytic upgrading of fractionated lignocellulose, synthesis gas route to fuels and chemicals.

Market, overall expected impact: Developing potential cascade chemical processes using functionalised catalysts is essential towards a viable and biomass valorisation to a large variety of bio-based products. Advances in catalysis and materials science provided innovative strategies for the design of catalytic materials with well-defined structures and special characteristics for efficient biomass upgrading. In regard to the associated market potential for bio-based chemicals and materials, please refer to '**Chapter 2**: 'Bio-based chemicals and materials (**2.3**)'. Regarding Horizon Europe (HEU) (see **3.9)**, there is an expected impact via:

- **Developing energy efficient catalytic processes** to enable commercialisation of biomass-to-fuels and biomass-to-chemicals pathways;
- **Broadening the biomass feedstock portfolio through viable processing of a wider range of feedstock** (including biomass residues), accounting for composition variability in different types of feedstock and compositions;
- **Strengthening bioeconomy competitiveness**, through **broadening** the **bio-based products portfolio** through selective catalytic processes to produce both drop-in but also dedicated structure products.

Horizontal challenges:

- Catalyst or biocatalyst stability against poisoning and coke precursors which may be present in biomass-based feeds;
- Catalysts with improved properties (noble metals free, no leaching) through rational design;
- New catalysts and routes for preventing the formation and processing of by-products from biomass conversion (e.g. black liquor);
- Improvement of efficiency, productivity and sustainability when compared to current benchmark processes;
- Process intensification and continuous processes are needed to reduce costs and environmental impact.

SUSCHEM PILLARS – MULTI-KETS:

Enhancing biomass catalytic valorisation is expected to have impact on RD&I in **Advanced Materials (Chapter 2)** and especially on 'Bio-based chemicals and materials (2.3)'.
The integrated reactor systems as well as catalyst design for biomass valorisation will be advanced through **Enabling Digital Technologies (Chapter 4)**, with a strong relevance of 'Laboratory 4.0/ Digital R&D (4.1)', 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation 4.3' but also 'Coordination and management of connected processes at different levels 4.8' due to supporting the connection between biomass suppliers and the chemical sector.

Within **Advanced Process Technologies (Chapter 3)**, links should be made, mainly, with 'Tolerant and Intensified Reactors and Processes - feedstock variability (3.1.1)', 'Membrane reactors - integrated systems (3.16)', 'Batch-to-continuous: Flow Chemistry (3.1.4)', 'Modular production (3.2)', 'Separation technologies (3.3)', 'Electrochemical, Electrocatalytic and Photo electrocatalytic processes (3.5)', 'Bioprocess development (biomass and waste valorisation) (3.10.3)' and 'Waste valorisation process technologies 3.11'.

RD&I Actions

3.9.1.1 Catalysis in biomass liquefaction

Context: Lignocellulosic biomass can be liquefied by pyrolysis processes or hydrothermal liquefaction (HTL). Both processes can be enhanced by catalysis. Catalytic technologies need to tolerate/utilise oxygen given that the biomass feedstock is oxygen-rich (e.g. catalytic pyrolysis to aromatics and bio-based solvents). Homogeneous base catalysts are the most typical catalysts applied in HTL whereas acidic zeolites are widely used for catalytic fast pyrolysis (CFP). Recently, some further modifications of these processes with enhanced performances have been reported e.g. hydropyrolysis where hydrogen and supported metal catalysts are applied in the conditions of fast pyrolysis. In this process, conditions are close to oil refinery hydrocracking processes.
Bio-oil from liquefaction is a complex stream with typically hundreds of different monomeric and oligomeric compounds. To utilise this stream for transportation fuels or chemical applications, heavy upgrading is typically needed. To produce fuels, this typically means multi-step catalytic hydrodeoxygenation (HDO) and further upgrading (hydroisomerisation, hydrocracking) at oil refineries. Targeting the production of chemicals from bio-oils is even more challenging due to the complex chemical nature of these oils.

Specific challenges:

- Low bio-oil yields and low catalyst tolerance against poisons in fast pyrolysis (catalyst regeneration issue);
- Impact of solid catalysts in hydrothermal liquefaction (HTL);
- Catalyst deactivation in bio-oil upgrading to fuels by hydrodeoxygenation (HDO);
- Conversion of bio-oils to chemicals.

Specific expected impact: Catalysis in biomass liquefaction will achieve a significant impact on realising large-scale implementation of advanced biofuels production technologies, as well as developing new sustainable routes to platform and specialty chemicals and new circular economy routes from biomass waste.

IMPACT EXAMPLES:

Example 1: Demonstrating HTL conversion compatibility with diverse advanced biomass feedstocks (grass Miscanthus, Microalgae, sewage sludge), achieving a heat recovery rate of 80 % and average yields of 26 wt %, 33 wt % and 25 wt % respectively from miscanthus, spirulina and sewage sludge. The corresponding chemical energy recovery in the biocrudes was 48 %, 47 % and 34 %.[174]

TRL(now) & TRL(2030): TRL of liquefaction routes enhanced by solid catalysts or by bio-oil upgrading is currently at TRL 3-5, more demonstration activities to reach a TRL 7-9 by 2030 is needed.

3.9.1.2 Catalytic upgrading of fractionated lignocellulose

Context: Lignocellulosic biomass can be fractionated by hydrolysis processes and the obtained fractions, lignin, cellulose and hemicellulose, can be converted to chemicals and fuel components by catalytic processes. However, only few of these processes are at a commercial stage. Of biomass fractions, conversion of lignin is the most challenging due to its complex chemical structure and high reactivity. The most successful has been so far to develop processes where the lignin oligomeric structure has been preserved whereas processes based on lignin depolymerisation are still at low TRLs. However, there are plenty of publications e.g. on lignin catalytic depolymerisation applying hydrogenolysis or solvolysis over supported metal catalysts. The processes from pentose and hexose sugars obtained from cellulose and hemicellulose hydrolysis are typically based on catalytic modifications of these sugars or acid catalysed dehydration of the sugars to furfural and 5-hydroxymethylfurfural (5-HMF). Furfural or 5-HMF can be further converted e.g. by catalytic hydrotreament or oxidation to specialty chemicals or fuel components.

Specific challenges:

- Depolymerisation of lignin to monoaromatics is still a quite low TRL technology;
- Selectivity of catalytic routes from furfural and 5-HMF to high-value chemicals, due to high reactivity of furfural and 5-HMF. For example, by-products (humins etc.) are formed in acid catalysed dehydration of sugars to furfural and 5-HMF. The long-term stability of the catalyst in these processes must be optimised.

Specific expected impact: Catalytic upgrading of fractionated lignocellulose will achieve a significant impact on enabling new sustainable routes to (i) establish process routes from biomass waste, (ii) enable the production of base and specialty chemicals and polymers, and (iii) facilitate the production of high-performance fuel components (e.g. 2MF, DMF).

IMPACT EXAMPLES:

Example 1: Development of a catalytic route, using a tandem electrocatalytic reactor (TER) coupling an oxidation reaction to a reduction reaction, in a process intensification strategy. The process is applicable to the conversion of sugars to 2,5-furandicarboxylic acid (FDCA), an intermediate to produce polyethylene furanaote (PEF): a next-generation 100 % renewable plastic.[175]

TRL(now) & TRL(2030): TRL depends on application areas. For example, catalytic upgrading of fractionated lignocellulose, based on sugars dehydration over solid acid catalysts is currently at TRL 4-5, demonstration activities to achieve a TRL 7-8 by 2030 need to be supported. Furfural and HMF conversion by catalytic hydrotreatment and oxidation is currently at TRL 2-3, demonstration activities to achieve a TRL 6-8 by 2030 need to be supported. Catalytic upgrading from sugars to monomers is currently at TRL 4-6, and a TRL >7 could be reached by 2030 upon further RD&I activities.

3.9.1.3 Biomass to synthesis gas - routes to fuels and chemicals

Context: Gasification and purification of gas from fossil raw materials as well as conversion of synthesis gas to a large variety of fuels and chemicals is a well-established technology. In principle, syngas reactions are not dependent on the raw material, but relevant differences still exist when using biomass as feedstock and several challenges still must be addressed. Despite the challenges, it should be highlighted that high-quality fuels and chemicals can be obtained from a large variety of different types of biomass. Technologies to be developed include:

- **i)** Biomass-to-liquids (BTL) route to Fischer-Tropsch diesel and jet-fuel;
- **ii)** Biomass-to-methanol and to a variety of chemicals from methanol;
- **iii)** Biomass-to-olefins either through methanol (MTO) or via Fischer-Tropsch reaction (FTO).

Specific challenges:

- There is less experience of biomass gasification. Biomass gasification plants are, due to logistics and technical restrictions, one order of magnitude smaller than coal or natural gas plants. There is a need to find feasible methods for gas purification and product upgrading at the small scale, suitable also for decentralised production;
- The impurity levels in the gas are different. For instance, the level of sulphur in biomass gasification gas is typically 100 ppm which is not a high value, but still much more than catalysts can tolerate;
- H/C-ratio in biomass is generally low and the share of hydrogen needs to be increased for most applications;
- Diversify gasification feedstock to include many types of woody residues, straw and other agricultural residues as well as various waste-derived;
- Reduce the investment cost of the plant (CAPEX).

Specific expected impact: Synthesis gas routes are to achieve a significant impact on producing chemicals such as methanol, olefins and aromatics produced from biomass-derived synthesis gas.

IMPACT EXAMPLES:

Example 1: The production of biofuels from solid biomass involves several steps: gasification of biomass, cleaning of gasification gas to useful synthesis gas, production of raw biofuel by Fischer-Tropsch synthesis and upgrading the product to transportation fuels. The development of a novel biomass-to-liquids (BTL) production plant reduced biofuel production costs up to 35 % compared to other routes. The production concept is based on distributed primary conversion of various kinds of biomass residues to intermediate liquid products with a capacity of 50 kt/a, based on a simplified gasification and Fischer–Tropsch process scheme. The specific investment costs of the plant are €3 million/ktoe and the production cost of biodiesel is reduced to €0.80 /l. The primary conversion will be integrated into local heat and power production resulting in 80 % energy efficiency in biomass utilisation.[176]

TRL(now) & TRL(2030): TRL of synthesis gas routes is currently at TRL 4-5, more demonstration activities to reach a TRL 5-6 by 2030 needs to be achieved.

3.9.2 Enabling waste valorisation via catalysis

Context: More robust and energy efficient catalytic processes need to be developed to ensure the efficient valorisation of waste to produce fuels and platform chemicals in the frame of the circular economy. Advances in catalysis will thus enhance the feasibility of handling feedstock variability, a key challenge under the circular economy. RD&I actions should address innovative catalytic processes, either in the conversion process itself or in post-treatment to efficiently convert waste to high- value products, based on different types of waste and especially plastics waste. In this context, a major technology priority is thermocatalytic cracking of plastics.

Market, overall expected impact: In 2018, 29.1 million tonnes of plastic waste were collected in Europe of which 24.9 % was still sent to landfill, leading to a loss of valuable resources.[177] About 32.5 % entered recycling facilities and 42.6 % were treated for energy recovery.[178] If plastics demand follows its current trajectory, global plastics waste volumes would grow from 260 million tons per year in 2016 to 460 million tons per year by 2030, presenting a great challenge and an opportunity for plastics waste to be used as alternative feedstock [179]. Technology options include mechanical, chemical and biotechnological recycling, and combinations thereof. Regarding advanced processes for waste valorisation, please also refer to 'Waste valorisation process technologies 3.11'.

Regarding Horizon Europe (HEU) (see **3.9**), there is an expected impact via:

- **Demonstrating incre ased opportunities and reduced risks upon scaling-up recycling and valorisation processes applicable to plastics waste**;
- **Developing robust and energy efficient catalytic processes** to enable commercialisation of plastics waste to fuels and chemicals, tackling the feedstock composition variability;
- **Enhanced access to affordable and secure energy as well as increased competitiveness of the European industry** through diversification of feedstock for energy and chemicals.

Horizontal challenges:

- Increase catalyst robustness given the fluctuation and diversity of plastics waste as feedstock for selective catalytic conversion processes by combining the physicochemical characterisation of the waste and a knowledge-based approach development of all process steps;
- Catalytic processes should be focused on selectivity, large operating window, stability, loading of the selected catalysts and regeneration potential.

SUSCHEM PILLARS – MULTI-KETS:

Enabling waste valorisation via catalysis will be supported by 'Additives for sorting, tracking and separation (2.4.1)', outlined under **Advanced Materials (Chapter 2)**.

Enabling Digital Technologies (Chapter 4) facilitate catalyst design for waste valorisation with a strong relevance of 'Laboratory 4.0/ Digital R&D (4.1)' and 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation 4.3' but also 'Coordination and management of connected processes at different levels 4.8' due to supporting the connection between the waste management sector and the chemical sector

Within **Advanced Process Technologies (Chapter 3)**, links should be made, mainly, with 'Tolerant and Intensified Reactors and Processes - feedstock variability (3.1.1)', 'Batch-to-continuous: Flow Chemistry (3.1.4)', 'Separation technologies (3.3)' and 'Chemical recycling of plastics waste (3.11.1)'.

RD&I Actions

3.9.2.1 Thermocatalytic cracking of plastics waste

Context: Currently, there is a need to boost recycling solutions for plastic-containing complex waste streams or develop new approaches, including sustainable options for chemical recycling technologies. Thermochemical conversion could be one answer to this dilemma as it poses a necessary contribution to converting organic and plastic-rich complex waste feedstocks into secondary resources, in those cases where direct reuse or mechanical recycling are not viable. Gasification and cracking (thermal pyrolysis, catalytic pyrolysis and hydrocracking) are the most important conversion technologies amongst many different approaches used for feedstock recycling.

Specific challenges:
Please refer to '(**3.11.1a**) Chemical recycling of plastics waste by pyrolysis' and '(**3.11.1b**) Chemical recycling of plastics waste by gasification'.

Specific expected impact: Please refer to Market, overall expected impact (**3.9.2**).

IMPACT EXAMPLES:

Example 1: Thermal cracking of polypropylene (PP) and low-density polyethylene (LDPE) in a reactor, achieving a total conversion of the polymers to liquid of about 86 wt % for PP and 94 wt % for LDPE.[180]

Example 2: Effective conversion of waste plastics to gasoline range hydrocarbons through a two-stage pyrolysis-catalysis using MCM41 and then ZSM-5, achieving 83.15 wt % yield at 1:1 ratio with high aromatic content.[181]

TRL(now) & TRL(2030): Thermocatalytic cracking of plastics is currently at TRL 3-4, more demonstration activities to reach a TRL 5-6 by 2030 need to be supported.

3.9.3 Enabling CO_2 valorisation via catalysis

Context: CO_2 (and CO from industrial waste gases) can be considered as an alternative and abundant carbon source to produce polymers and chemicals including energy carriers with a lower environmental footprint compared to standard production routes. Various technologies such as thermocatalytic, electrocatalytic, photocatalytic, biotechnology routes or plasma technologies are considered for the chemical valorisation of CO_2 to target molecules. Catalysis plays an essential role in the chemical valorisation of CO_2 which has very low energy content and low reactivity.

Market, overall expected impact:
The catalytic utilisation of CO_2 can allow the production of a wide range of chemicals, from base chemicals to fine chemicals and polymers with a lower carbon footprint. Additionally, the production of syngas or bulk chemicals from CO_2 can play a key role in the introduction of renewable electricity in the chemical industry and CO_2 emissions reduction. The valorisation of CO_2 through Power-to-X technologies can also provide solutions for renewable electricity storage and the production of low-carbon fuels. Regarding Horizon Europe (HEU) (see **3.9**), there is an expected impact via:

- Enabling the **valorisation of CO_2 as an alternative carbon feedstock**, contributing to a more circular economy through recycling of carbon from CO_2;
- **Contributing to the development of a low-carbon economy** via the introduction of renewable energy in the chemical industry in particular through power-to-chemicals, electrocatalytic and electro photocatalytic CO_2 valorisation routes;
- Providing options for **renewable energy storage** through 'power-to-chemicals' technologies.

Horizontal challenges
- Development of highly active/efficient and selective catalysts given the low reactivity of the CO_2 substrate;
- Development of catalysts less prone to poisoning enabling the utilisation of less purified CO_2 streams;
- Catalysts enabling CO_2 valorisation processes at lower temperature and/or pressure;
- New heterogeneous and homogeneous catalyst for direct CO_2-to-chemicals and polymers;
- Catalysts for direct CO_2 electrochemical and photo electrochemical reduction reactions;
- Development of catalysts based on abundant metals.

SUSCHEM PILLARS – MULTI-KETS:

There is a horizontal dimension of E**nabling Digital Technologies (Chapter 4)** to enable the development of catalysis for CO_2 valorisation, in particular 'Laboratory 4.0 - Digital R&D (4.1)' and 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation 4.3'.

Catalysis for CO_2 conversions can benefit from other **Advanced Process Technologies (Chapter 3)** 'New reactor design and equipment (3.1)', 'Modular production 4.2' and 'Plasma-based process technologies (3.4.1)', and will impact 'Electrochemical, Electrocatalytic and Photo electrocatalytic processes (3.5)' and 'Power-to-chemicals (3.8)'.

RD&I Actions

3.9.3.1 Thermocatalytic valorisation of CO_2

Context: Thermocatalytic processes are currently the most developed routes from CO_2 to chemical intermediates and fuels, as well as for direct production of polymers from CO_2. However, there are still challenges to be solved in particular to enable operation with less purified feed streams with catalysts more tolerant to impurities.

CO_2-to-C1 molecules through hydrogen-based route
Catalytic conversion processes for CO_2 to C1 molecules, via power-to-chemicals, are at high TRL processes and are based on heterogeneous supported metal catalysts. Current power-to-methanol processes use syngas, produced by electrolysis of water and CO_2 and Cu-ZnO-catalysts supported on Al_2O_3 to produce methanol. The operation of the catalytic reaction takes place at pressures >70bar and temperatures below 250°C. These conditions help to stabilise the catalyst but result in low conversion rates. Catalyst development to increase the stability, selectivity and the tolerance towards water are needed. Methanation of carbon dioxide and hydrogen to methane at temperatures between 300 and 600 °C at moderate pressures with Ni-containing catalysts. The catalyst design has to be improved for operation at lower temperatures, with increased activity and tolerance to poisoning.

CO_2-to-hydrocarbons

Current industrial Fischer-Tropsh (FT) processes for CO_2 to hydrocarbons uses Co and Fe based catalysts. For a decentralised operation, the reactors need to be smaller and the exothermicity of the reaction needs to be better controlled. Therefore, catalysts need to be developed that operate at lower temperatures with higher selectivity.

CO_2-to-polymers

CO_2 can be used as an alternative carbon source to produce polymers through two major chemical routes:

- **i)** either indirectly, by utilising intermediates obtained by chemical valorisation of CO_2 (e.g. CO_2-derived olefins, CO_2-derived non olefinic intermediates), or
- **ii)** by utilising directly CO_2 as co-monomer with co-reactant to produce polymer (e.g. copolymerisation of CO_2 with epoxides to polyols or poly(propylene)carbonate). Such CO_2 valorisation routes do not require hydrogen.

Specific challenges:

- Catalyst selectivity and efficiency;
- Catalyst tolerance against impurities from CO_2 feed streams;
- Catalyst for operations at lower temperature (including for Fischer-Tropsch and methanation);
- Catalyst for one step conversion of CO_2 to hydrocarbons (e.g. direct FT of CO_2 without reverse water-gas shift (RWGS) step);
- Catalyst for direct processes from CO_2 to-chemicals and polymers;
- New catalysts for new polymer structures with novel properties;
- Catalyst removal and recovery, where needed.

Specific expected impact: Thermocatalytic valorisation of CO_2 can enable large scale production of chemical building blocks from CO_2, with significant GHG emissions reduction in the chemical sector, providing competitive access to low-carbon hydrogen. A recent study estimated CO_2 emissions reduction of 30 million t CO_2 /y in 2050 in an ambitious deployment scenario of CO_2-to-methanol and methanol-to-olefins in Europe.[182] In addition, thermocatalysts for the direct conversion of CO_2 to polymers can effectively contribute to carbon circularity and a lower environmental footprint of polymer production. New catalysts can enable new polymer structures with novel properties.

IMPACT EXAMPLES:

Example 1: Producing methanol from CO_2 and H_2 from renewable electricity, with a reduction of 90 % regarding CO_2 emissions when compared to the fossil-based production route.[183]

Example 2: Development of new catalyst and process to produce polyurethane intermediates from CO_2 and CO from steel production, for a reduction of the carbon footprint of 20-60 % compared to today's polyurethane product and saving 70 % of process energy vs. conventional production.[184]

TRL(now) & TRL(2030): TRL of catalytic routes from CO_2 to methane or methane and FT hydrocarbons (two-step process) is currently 5-7 and could reach 8-9 by 2030. The TRL of direct FT from CO_2 to hydrocarbons is currently at 2-3 and could achieve TRL 6-7 by 2030. The direct routes from CO_2-to -chemicals have typically currently TRL 1-4 and are expected to reach TRL 5-7 by 2030. For CO_2-to-polymers a first polyol demonstration plant has been built, but development for other types of polyols and polymers are at lower TRL.

3.9.3.2 Electro-catalytic and photo electrocatalytic valorisation of CO_2

Context: The reduction of CO_2 via electrocatalysis can enable the direct production of chemicals (including C_{n+1} molecules) from CO_2, independent of the availability of low-carbon hydrogen. Such technologies offer low-carbon options to produce chemicals (e.g. formic acid, oxalic acid, dimethyl ether (DME) through the direct introduction of low-carbon electricity in chemical processes and contribute to reduce the emissions from the chemical industry. For electro photocatalysis at least one of the electrodes is photoreactive, which enables reduced energy requirement compared to electrocatalysis.

Specific challenges

- Highly active/efficient and selective catalysts are needed;
- Catalysts less prone to poisoning enabling the utilisation of less purified CO_2 streams;
- Catalysts enabling CO_2 valorisation processes at lower temperature and/or pressure;
- Catalysts enabling the robustness of continuous processes under relevant operation conditions;
- Avoid or minimise further steps of conversion to produce final chemicals/fuels, consider the scalability and use of electrochemical devices, avoiding the use of critical raw materials;
- Catalyst removal and recovery, where needed.

IMPACT EXAMPLES:

Example 1: Development of a combined electrochemical technology for the simultaneous conversion of CO_2 to ethylene at the cathode, water oxidation to hydrogen peroxide at the anode and a subsequent chemical conversion of both intermediates to ethylene oxide and oligo-/polyethylene glycol in a cascade.[185]

Example 2: Design and optimisation of a photo-electro-catalytic (PEC) cell prototype for the production fuels and chemicals using CO_2, water and solar energy aiming at 10 % efficiency, using ultra-thin layers and nanoparticles of metal or metal oxide catalysts for both half-cell reactions.[186]

TRL(now) & TRL(2030): Some electrochemical technologies for the conversion of CO_2 to C(n+1) target molecules (formic acid, oxalic acid and other chemicals) are at TRL 3-4. CO_2 to ethylene through electro-catalytic process is currently investigated at lab scale. Photo electrochemical reactors are currently at TRL 2-4. More demonstration activities to explore new designs to achieve at least TRL 5-7 by 2030 need to be undertaken.

3.9.4 Light hydrocarbons catalytic valorisation

Context: The development of novel catalytic routes for the valorisation of currently unexploited light hydrocarbons resources is thought to broaden the range of feedstock for chemical and energy production, from the perspective of energy transition. In all cases, it is necessary to develop the catalysts and process engineering which validate the feasibility of the proposed route in industrial relevant environments, including the scalable synthesis of catalysts and the analysis of the costs/benefits with respect to the actual routes. Based on better understanding on C-H and C-C activation and catalyst deactivation, the rational design of the catalysts should allow broadening the use and applications of project results beyond case studies. The main technology priority included is direct catalytic conversion of light hydrocarbons.

Market, overall expected impact: In the context of the low carbon economy, increasing the exploitation of natural gas, stranded resources and biogas creates new opportunities for the utilisation of low-cost light alkanes. High value can be added through improved catalytic transformations to C2-C4 olefins, aromatics, C-C coupling and/or C1 chemistry, integrating catalysts and process design.
Regarding expected impact on Horizon Europe (HEU) (see **3.9**).

Horizontal challenges:

- More robust, selective, flexible and aging-resistant catalysts and catalytic processes will allow to better handle feedstock variability;
- Scalable catalyst manufacture with reduction of the consumption of critical raw materials and preferably starting from earth-abundant and accessible raw materials.

SUSCHEM PILLARS – MULTI-KETS:

There is a horizontal dimension of **Enabling Digital Technologies (Chapter 4)** to enable the light hydrocarbons catalytic valorisation, in particular 'Laboratory 4.0 - Digital R&D (4.1)' and 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation 4.3'.

Light hydrocarbons catalytic valorisation can benefit from other **Advanced Process Technologies (Chapter 3)** 'New reactor design and equipment (3.1)', 'Modular production (3.2)', 'Separation process technologies (3.3)' and 'Industrial biotechnology 3.10'.

RD&I Actions

3.9.4.1 Direct conversion of light hydrocarbons

Context: There are very large resources of light hydrocarbons (C1-C4 alkanes), especially methane, which are not efficiently utilised as raw material for fuels or chemicals. Examples of these resources include stranded natural gas, shale gas, biogas and many industrial gas streams. Currently, these gases are largely unused and flared or vented into atmosphere. An example of a valuable stream is coke oven gas, a side product of steel industry, which mainly consists of 25-30 % methane together with hydrogen and a small percentage of carbon monoxide, carbon and nitrogen. Technologies suggested for the direct conversion include:

- Conversion of C2-C4 hydrocarbons to olefins and butadiene;
- Conversion of non-transportable methane resources to ethane, ethylene and possibly liquid hydrocarbons;
- New energy-efficient and cost-competitive routes for the direct utilisation of light alkanes in the production of aromatics and other high-value chemicals.

Specific challenges:

- Methane is a very stable compound and the direct coupling to ethane and ethylene has proven to be challenging. The achieved yields of oxidative methane coupling have often been very limited as the reactivity of the products is much higher than that of methane. On the other hand, the non-oxidative coupling of methane is thermodynamically highly unfavourable but offers reasonably good selectivity. The thermo-dynamic limitation makes the activity extremely low and the two-step process operating at different reaction temperatures is difficult to operate industrially;
- C2-C4-hydrocarbons are much more reactive than methane but improved performance on reaction metrics and cost competitiveness compared to existing industrial processes is needed;
- The light hydrocarbons are seldom available as pure compounds in high concentrations, which are directly suitable for catalytic conversion, therefore efficient gas cleaning and upgrading technologies are needed;
- Efficient technology suitable for the separation and purification of gas streams to make them fit for catalytic conversion. Technology for both decentralised (such as biogas) and large-scale production (e.g. coke oven gases from steel production).

Specific expected impact: See **Market, overall expected impact (3.9.4)**.

IMPACT EXAMPLES:

Example 1: Decentralised production of chemicals and liquid fuels, for which monetary savings of more than 10 % are expected. The process involved the conversion of methane to C2+ hydrocarbons, based on intensified adaptable catalytic reactor systems for flexible and decentralised production at high process performance, able to operate with changing feedstock composition and deliver "on-demand" the required product distribution by switching selected operational/control parameters and/or changing modular catalyst cartridges.[187]

TRL(now) & TRL(2030): The catalytic technology for converting methane to products has currently a low TRL of 2–3 and a move to TRL 4-5 by 2030 is expected. The conversion of other light alkanes (C2-C4) to products has slightly higher TRL (3–5) and a move to TRL 5-6 by 2030 should be aimed at.

3.10 Advanced Processes: Industrial Biotechnology

Context: Industrial Biotechnology (IB) encompasses cross-disciplinary technologies that use renewable and biological resources to produce platform chemicals, biosurfactants, advanced biofuels, alternative food-related products and materials, with potential in a wide range of sectors. It contributes to industrial competitiveness, by also facilitating advanced processes and new products.

However, IB-based processes are at a less mature stage of development relative to conventional chemical processes; hence further RD&I is required to drive scalability. Optimised biotech processes offer benefits in terms of novel product functions, improved resource and energy efficiency, and process safety. Recent progress in genetic tools (e. g. bioinformatics, genome editing) fuel the expectation of rapid progress in the development of industrially relevant microbial strains at a European level as well.
Key horizontal challenges for IB advanced processes encompass scaling-up and low productivity due to improvements required in upstream and downstream processes, including separation and purification developments. Overall, innovation priorities include **engineering of microorganisms and enzymes, and bioprocess development, especially for the valorisation of biomass and/or waste.**

Market, overall expected impact:
Industrial biotech, when considering direct, upstream and downstream employment, has close to 500,000 jobs in the value chain and more than €31 billion is generated in terms of value added. It is a sector with significant growth potential, and in 2030 employment in the industrial biotech value chain may increase to well above one million jobs, contributing up to €99.5 billion to the EU economy.[188] With advanced biotech processes contributing to bioeconomy and circular economy and a range of products, IB becomes increasingly important to finding solutions that help meet different UN SDGs.[189]

Industrial biotechnology-based advanced processes address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Energy supply' 5.2, 'Clean, safe and accessible transport and mobility' (5.7), 'Energy storage' (5.9), 'Biodiversity and natural resources' (6.2), 'Agriculture, Forestry and rural areas' (6.3), 'Seas, Oceans and inland waters' (6.4), 'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7), with additional impact on Cluster 1: 'Health'.

3.10.1 Engineering of microorganisms and enzymes (in silico and in vitro)

Context: The rising relevance of microorganisms and microbial products in end-use industries and recent advances in biotech have expanded the prospects of engineering microorganisms, thereby creating novel market avenues. Technology priorities in this area encompass, amongst others: engineering and bioprospecting industrial microbial hosts tolerant to extreme habitats, the combination of metabolic engineering (model-based) experiments and process engineering as well as in vitro synthetic biology for biomanufacturing.

Market, overall expected impact: Engineering of microorganisms and enzymes shows promise to further improve efficiency of biotech processes, with a global market size of approximately $8 billion in 2016, and a CAGR of 7.2 % over the period 2017-2025.[190] Regarding Horizon Europe (HEU) (see **3.10**), there is an expected impact via:

- **Improved flexibility in biotech processes** by developing robust industrial 'microbial factories' to produce a wide range of products;
- **Novel products** by integrating metabolic engineering with process engineering. This includes the sustainable production of novel products to enhance human and environmental health;
- **Enabling the valorisation of alternative carbon feedstock**, i.e. robust enzymes or bacteria to produce chemicals and fuels from waste and/or biomass.

Horizontal challenges:

- Adapting microorganisms to process conditions implies inverting the state-of-the-art paradigm of process adaption to microorganisms.

SUSCHEM PILLARS – MULTI-KETS:

Engineering of microorganisms and enzymes (in silico and in vitro) is expected to have impact on RD&I in **Advanced Materials (Chapter 2)** and especially on 'Bio-based chemicals and materials (2.3)'.

Engineering of microorganisms and enzymes will be strongly supported by **Enabling Digital Technologies (Chapter 4)**, with a relevance of 'Laboratory 4.0/ Digital R&D (4.1)', 'Process

Analytical Technologies (PAT) 4.2', 'Advanced data analytics and artificial intelligence 4.4' and 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation 4.3'.

Within **Advanced Process Technologies**, links should be made, mainly, with 'Catalysis (3.9)' and 'Waste valorisation process technologies 3.11'.

RD&I Actions

3.10.1.1 Engineering and bioprospecting industrial microbial hosts tolerant to extreme habitats

Context: Industrial Microbial (IM) Hosts are the production 'factories' for almost all industrial biotechnological processes by being directly involved in product formation or indirectly involved by producing essential intermediates or catalysts to enable production. IM hosts require a minimum set of process-dependent properties such as suitable feedstock to more advanced properties, e.g. compatible regulatory networks, adjustable metabolic fluxes or cell robustness. Relative to the number of microbial species and the diversity and properties contained therein,[191] the industrially used microbial species represent a very small fraction of the available capabilities. The low diversity approach to IM Hosts allows the use of well-characterised microorganisms with established cultivation methods and high process-application success. However, this significantly decreases process flexibility, essential to efficient commercial production. Currently, process conditions are determined by the IM host, thus limiting the achievable process efficiency and the range of products possible. Process conditions barriers include: pH, alternative solvents, substrate and product concentrations, high/low pressures, hygiene requirements and security considerations.

Specific challenges:

- Process-centred strain engineering of and bioprospecting for IM Hosts;
- Metabolic engineering of industrial platform microorganisms;
- Address the efficient use of mixed carbon sources;
- Omics and bioinformatics to understand and apply the natural properties to IM Hosts;
- Engineering IM Hosts tolerant to variable conditions/ extreme habitats (including pH/solvent/toxins/ pressure).

Specific expected impact: With the advent of modern biotechnological tools, the paradigm of IM Host-dependent processes can be reversed to process-dependent hosts, selected and evolved for the process conditions. Thus, IM Hosts are to achieve a significant impact on increasing the effectiveness and scope of IB in a wide range of applications including Active Pharmaceutical Ingredients (APIs), platform and specialty chemicals and biofuels.

IMPACT EXAMPLES:

Example 1: Development of Pseudomonas putida strains with improved adenosine triphosphate (ATP) availability, able to produce new active ingredients for crop protection, providing strong versatility, enhanced efficiency and efficacy to the production processes.[192]

Example 2: Development of a new generation of super-producing microbial hosts, contributing to the production of recombinant proteins, particularly biotherapeutics and industrial enzymes, critical products of the EU biotech sector.[193]

TRL(now) & TRL(2030): Few strains (*e.g. Escherichia coli, Bacillus, Actinomycetes, Pseudomonas* and lactic acid bacteria) are currently at TRL 8-9. For other strains currently at TRL 3-5, more research and demo activities are recommended to go from lab to piloting (TRL 7-8) by 2030.

3.10.1.2 Combine metabolic engineering (model-based) and process engineering

Context: To develop industrially relevant microorganism strains, metabolic engineering and process development must go hand-in-hand. Recent progresses in genetic tools, bioinformatics and machine learning enable a better integration of metabolic engineering with process engineering. This is expected to reduce time-to-market and enable a cost competitive position for the EU for producing novel or established products in industries like consumer goods, nutrition, or cosmetics.

Specific challenges:

- Automated or assisted structuring and linking of data along value chains. This includes metabolic engineering from strain genealogy and target selection in the lab, validation of data from test runs in pilots, and multi-variate assessment in production;
- Multi-Scale-Modelling of fermentation and downstream processing (DSP). A suitable solution will lead to a digital twin. Machine learning assisted data analysis of batches in (multi)scales;
- Model-Based process development to speed up development: validate process models in industrially relevant scale (e.g. validate computational fluid dynamics (CFD) models) as a base for requirement

definition for metabolic engineering and subsequent model-based experiments;
- Advanced data analytics in R&D results interpretation, especially for fermentation and DSP;
- Deep learning algorithms for accelerated DoE to minimise and shorten the Design of Experiments .

3.10.1.3 In-vitro Synthetic Biology for biomanufacturing

Context: Synthetic biology, described as "making biology easier to engineer"[194], is highly promising for delivering high levels of product yield, coupled with atom economy and minimal by-products. It is also a needed tool to meet consumer expectations of "smart" molecules and materials for e.g. precision medical treatments, or prebiotic nutrients. Synthetic biology has been advancing fast in vivo, but it is necessary to design cell-free[195] in vitro platforms for viable biomanufacturing.[196] This reduces non-linear kinetic effects characteristic of cell-driven bioreactors as well as avoiding regulatory restrictions[197] arising from the direct use in a manufacturing process of genetically enhanced microbes. The practicability of such in vitro manufacturing has been shown.[198]

Specific challenges:
- Combine synthetic biological methods coupled with state-of-the-art chemical synthesis for the sustainable manufacture of specialty molecules and polymers by utilising enzymes designed using mutagenic techniques, coupled where necessary with novel chemo-catalysts;
- Further research on demo projects comprising modular biomanufacturing, analogous to the former F^3 Factory,[199] but concerning in vitro synthetic biology processes;
- Bring together cross-disciplinary and cross-sector investigators to support the actions above, in particular the required informatics and metrology (e.g. soft sensors to monitor product quality) and the development of one-pot multi-enzyme synthesis protocols.

3.10.2 Bioprocess development (upstream & downstream)

Context: Bioprocessing uses complete living cells or their constituents, ranging from whole bacteria to enzymes, to obtain desired products. Bioprocess development technology priorities encompass, amongst others: continuous flow bioprocessing at industrial scale, gas phase fermentations, process intensification to increase the industrialisation of IB and process intensification in biogas production to enable a better use of dilute waste.

Market, overall expected impact: Bioprocess development highly contributes to further improve the techno-economic performance and overall sustainability of biotech processes-based production of bulk chemicals, fine chemicals and fuels, including the valorisation of alternative feedstock (see **3.10** for relevance to Horizon Europe (HEU)).

Horizontal challenges:
- Low space time yield vs. transformation efficiency and low contamination necessitate process intensification where new reactor concepts are needed specifically for IB processes;
- High cost of biocatalysis applicable for processes for high price / low volume (specialty) but also low price / high volume (bulk) chemicals;
- Separation and purification technology developments specifically for IB;
- Enabling the automation and digitalisation of biotechnological processes.

SUSCHEM PILLARS – MULTI-KETS:

Bioprocess development is expected to have impact on RD&I in **Advanced Materials (Chapter 2)** and especially on 'Bio-based chemicals and materials (2.3)'.

All underlined priorities under **Enabling Digital Technologies (Chapter 4)**, will have a strong impact on bioprocess development.

Within **Advanced Process Technologies (Chapter 3)**, links should be made, mainly, with 'New reactor design concepts and equipment (3.1)', 'Separation process technologies (3.3)', 'Electrochemical reactors and processes (3.5.1)', 'Power-to-chemicals (3.8)', 'Catalysis (3.9)' and 'Waste valorisation process technologies 3.11', but also 'Engineering of microorganisms and enzymes (3.10.1)'.

RD&I Actions

3.10.2.1 Continuous flow bioprocessing

Context: Industrial biotechnology-based processes still face many challenges in comparison to the relatively mature chemical processes on industrial scale. An important technical challenge to overcome is the low space-time yield, a crucial factor for the higher costs of biotech products. Currently, most microbial bioprocesses are conducted in batch or fed-batch fermentations with a relatively low space-time yield. An opportunity to

increase the space-time yield is the switch to continuous bioprocesses. At present, continuous bioprocesses need to further be developed and optimised to become cost competitive and to reach industrial scale.

Specific challenges:

- Higher risk of contamination:
  - Feeding of raw materials and the removal of products in a continuous mode, without the risk of contamination;
  - Improve unsterile processes;
  - Reduce contamination in biotechnological processes without biocides or antibiotics;
- Robustness of the strain and stability of the biological system as a whole, during long cultivations. The selection criteria in strain development today do not reflect the demand for long term genetic stability under continuous flow conditions, which differ from batch and fed-batch conditions in terms of selection pressure in environment;
- Low production concentration should be addressed by different process design strategies for downstream, which may lead to changed process technologies (large volumes need to be processed downstream);
- Large-scale devices for retention of cells;
- New reactor concepts;
- Microorganisms that grow under special conditions (anaerobic, low pH or mixed culturing).

Specific expected impact: Continuous flow bioprocessing to achieve a significant impact on improving the costs competitiveness for bio-based specialties and intermediates in main areas including consumer goods, nutrition, and packaging.

IMPACT EXAMPLES:

Example 1: Bioconversion of solid municipal bio-waste fraction, and sludgy bio-waste from other industries, into H_2 and volatile fatty acids (VFAs) that are recovered continuously using advanced membranes. VFAs are then in turn used as feedstock / carbon source for value added-fermentation approaches such as biopolymers production, valuable in material applications.[200]

TRL(now) & TRL(2030): The development of continuous flow bioprocesses has achieved a TRL 3-5; more RD&I on demo and optimisation processes at TRL 6-8 needs to be considered by 2030. More fundamental research at TRL (1-5) would be in exploring new reactors to further reduce costs.

3.10.2.2 Fermentations with gas state substrate

Context: The area of gas fermentation is widespread and covers the usage of diverse gas-streams such as CO, CO_2, CH_4, and H_2 to produce chemical building blocks and fuels. These off-gas streams can originate from many industrial sectors such as chemical, refineries, steel-mills, ferro-alloy, agriculture and municipal waste treatment. Hence, gas fermentation offers the opportunity to produce products based on waste recycling. A different type of gas fermentation is the "Power-to-Gas concept" where CO_2 is converted to CH_4. For this one, reaching commercial scale production remains as a challenge as well. RD& I to gain speed and keep Europe competitive in this field is recommended.

Specific challenges:

- Development of appropriate microbial production strains meeting the industrial needs;
- High-efficiency fermentation reactors to manage the needed gas-liquid mass transfer;
- Integrated downstream processing concepts to achieve both optimum fermentation conditions and cost-effective downstream processing;
- Gases utilised are toxic and explosive, except for CO_2, making their handling challenging for pilot facilities, whilst downstream processing needs to be integrated into all scales of R& D.

Specific expected impact: Gas phase fermentations with gas state substrate to achieve significant impact on reducing GHG emissions and on valorising 'waste'.

IMPACT EXAMPLES:

Example 1: US-based companies currently operating the first commercial gas fermentation plants to produce bio-ethanol, achieving over 65 % lower GHG emissions via innovative biotech processing by valorising steel-mill off-gases from China.[201,202]

Example 2: Achieving a concentrated gas stream of at least 95 % CO_2 through using biotechnological processes to capture and convert CO_2 from industrial point sources, like refineries and cement production plants, into valuable platform chemicals, i.e. isobutene and lactate.[203]

TRL(now) & TRL(2030): The development of gas phase fermentations achieved TRL 5, more RD&I on demo and optimisation processes at TRL 6-8 needs to be considered by 2030. More fundamental research at TRL (1-5) would be on exploring reactor design to optimise fermentation processes.

3.10.2.3 Increased industrialisation of biotechnology processes via process intensification

Context: A key challenge of IB processes is low space-time yield due to low concentrations of substrate and product. This leads to inefficiencies and difficulties on multiple levels which in turn directly lead to increased waste, and high energy consumption due to the large reaction volumes or time in reactor. For example, the incomplete fermentation of lignocellulosic residues in 2G-bioethanol synthesis limit the space-time-yield; long reaction times increase the probability of contamination and increased use of biocontrol mechanisms, whereas low adduct concentrations lead to low product yields and the over proportional use of solvents. Process intensification would allow for a better industrialisation rate through increased efficiency, lower waste or higher space time yields.[204] An indirect decrease of the process duration can also reduce the probability of contamination and decrease or eliminate the need for biocides or antibiotics. Increasing process intensity will require a holistic approach to process design including new separation, purification and reactor concepts specifically tailored for IB, combined with the adaption of the biology to support intensified processes.

Specific challenges:

- Process centred engineering for biotechnology;
- Information- and model-based design and development;
- Biology supporting intensive process conditions;
- Intensification of processes using biomass and bio-waste.

Specific expected impact: Process intensification to lead to large efficiency increases in the pharmaceutical, fine chemicals and fuels towards first bulk production.[205]

IMPACT EXAMPLES:

Example 1: Two complementary lines developed in parallel, one focusing on biotechnology, based on improved yeast-strains, and one based on chemo-catalytic routes, included the testing of in-situ product recovery of selected products. Overall aiming to provide novel or optimised processes to convert sugars into added value compounds (drop-ins and novel bio-based chemicals).[206]

Example 2: Bringing together biotechnology scientists as well as microfluidic and modelling experts to make use of µ-technology and develop economically feasible intensified bioprocesses by integration of separation and process control, also creating tools to speed up the characterisation and assessment of different process technologies and biocatalysts.[207]

TRL(now) & TRL(2030): For some applications (e.g. production of chemicals and biofuels from waste or biomass) there are technologies currently at TRL 5. For those, more RD&I to reach TRL 6-8 needs to be considered by 2030. Technologies to produce biofuels from gases are at a lower TRL (1-5).

3.10.2.4 Process intensification in biogas production to enable a better use of dilute waste

Context: The basic technology for biogas production from biomass via anaerobic digestion has been developed over the past decades and has resulted in almost 18,000 biogas plants installed in Europe, with more than 50 % of them in Germany.[208] The broad variety of bio-waste feedstock applicable for fermentative biogas production - including agricultural waste, manure, sewage sludge and municipal waste - is a major reason why significantly increased biomethane production is considered a major element in a circular and climate neutral economy.

Specific challenges:

- Increasing the yield of biogas and accelerate digestion for better space-time-yields to achieve the ambitious production growth plans;
- Methane / biogas separation from aqueous digestion media is instantaneous and technically easy to achieve, making efficient use even of dilute waste streams. However, often digestion remains incomplete, in particular for lignocellulosic feedstock.

Specific expected impact: According to a 2019 JRC study, the EU annual production potential for biogas was 2 billion m^3/y (2017).[209] The same study expects an increase in biomethane production to 18 billion m^3/y by 2030, driven both by installation of new biogas plants and by upgrading of existing plants. Overall, biogas and biomethane will count towards the 32 % renewable energy share from EU energy consumption according to the revised Renewable Energy Directive.[210] This is to have an impact on reducing CO_2 emissions and increase the share of renewable energy.

IMPACT EXAMPLES:

Example 1: European biogas producers could achieve a combined €1 billion improvement in profitability while also cutting CO_2 emissions by 1.5 million tons and releasing 811,000 hectares of field for a more sustainable use such as food production with a technology capable of removing over 60 % of nitrogen from several organic waste materials for biogas production.[211]

TRL(now) & TRL(2030): Technologies for the production of biogas from diluted waste are currently at TRL 2-5, more RD&I on demonstration and optimisation at TRL 6-8 needs to be considered by 2030.

3.10.3 Bioprocess development (biomass and waste valorisation)

Context: Bioprocess development utilising biomass or waste encompass the following technology priorities, amongst others: biotechnological solutions to upgrade plant-based raw materials to alternative food products, the production of specialty carbohydrates and lipids, the development of novel products from undiscovered resources, as well as the production of bio-based polymers.

Market, overall expected impact: Around 1.3 billion t of food are wasted annually at a global scale, food that is originally produced under extensive use of energy and nutrients, not accounting the secondary sources of waste such as lignocellulosic biomass.[212] Regarding Horizon Europe (HEU) (see **3.10**), there is an expected impact via:

- Enabling the **valorisation of biomass and waste** to produce **chemicals** and **materials**;
- **Sustainable alternative food production** via biotech solutions;
- Sustainable production of **novel products** to **enhance human, animal and environmental health.**

Horizontal challenges:

- Adapt upstream and downstream processes to sustainable biomass feedstock availability;
- Ecoefficiency studies to identify optimal valorisation of biomass and waste feedstock;
- Develop and optimise viable processes for the conversion of biomass into substrates suitable for fermentation and bioconversion (e.g. enzymatic, physical, chemical, or a combination).

SUSCHEM PILLARS – MULTI-KETS:

Bioprocess development for valorising waste and biomass is expected to have impact on RD&I in **Advanced Materials (Chapter 2)** and especially on 'Bio-based chemicals and materials (2.3)'.

All underlined priorities under **Enabling Digital Technologies (Chapter 4)**, will have a strong impact on improving on the design and control of bioprocesses for waste and biomass valorisation.

Within **Advanced Process Technologies (Chapter 3)**, links should be made, mainly, with 'New reactor design concepts and equipment (3.1)', and especially 'Tolerant and Intensified Reactors and Processes – tolerance to feedstock variability (3.1.1)', 'Separation process technologies (3.3)', 'Catalysis (3.9)' and 'Waste valorisation process technologies 3.11' but also 'Bioprocess development (upstream & downstream) (3.10.2)' and 'Engineering of microorganisms and enzymes (3.10.1)'.

RD&I Actions

3.10.3.1 Biotech to upgrade plant-based raw materials as high-quality meat replacements

Context: The cost and environmental impact of animal farming, in particular raising cattle, is far higher than the production of plant protein; e.g. there are requirements of 3 kg of human-edible material, mostly grains and beans, to produce 1 kg of meat.[213] The need to nourish still more people on our planet whilst reducing our carbon footprint, increasing animal welfare, and also liberating more biomass for materials and energy makes the substitution of meat by plant protein a very high priority. However, changing human consumption habits will require further improvements of meat substitutes, including taste competitiveness. Biotech together with

food technology can become the key drivers to upgrade plant-based proteins and other raw materials to meet meat standards in taste and texture and leverage the cost and environmental advantages of plant derived food. While start-ups, especially in the US, have already taken pole positions in the technology race,[214] European R&DI needs an ambitious push to pave the way to eventually produce mainstream products.

Specific challenges:

- Define meat texture on molecular basis and find methods to give plant-based protein the same texture;
- Define aroma differences and produce the additives needed to close the taste gap (e.g. by fermented heme).

Specific expected impact: High quality meat replacements will achieve reducing water consumption, CO_2 emissions, and contribute to animal welfare.

IMPACT EXAMPLES:

Example 1: Enhanced protein production by 25 % through innovative, cost-effective and resource-efficient plant proteins from highly nutritious seed crops and legumes with high protein quantity, improving the quality of proteins and the sustainability of production and processing.[215]

TRL(now) & TRL(2030): Biotech to upgrade plant-based raw materials to quality meat replacements have achieved a relatively low TRL (1-5). More fundamental research at lower TRL would be on exploring meat textures and aromas, while generating novel and sustainable production processes. An ambitious target would be for plant derived meat replacements to be fully commercial by 2030.

3.10.3.2 Advanced processes and metrology for specialty carbohydrates and lipids

Context: Microbiome research on the effects of dysbiosis on human health has increased throughout Horizon 2020,[216] with research investments exceeding €600 million up to 2018.[217] Such research opened immense opportunities for modulating health through novel therapeutics and disease control, or by healthy eating linked to novel pro- and prebiotics. Advances in computing power coupled with metagenomics can now determine relative microbe populations in an individual, leading to the promise of precision medical and health treatments.

Carbohydrates are ubiquitous in acting directly to maintain a healthy microbiome but the speed of identification of suitable APIs or prebiotics and their progress to the market is hampered by a poor understanding of the complex mechanisms at molecular level. In addition, the synthesis of carbohydrates and glycans in high yields and with the right stereochemistry is a greater challenge than with other biomolecules[218] such as lipids. This requires improved metrological capabilities, coupled with databases, covering a range of –omics, but especially lipidomics and metabolomics due to possible interactions between lipids, carbohydrates and the microbiome. The large-scale production of specialty carbohydrates, glycans and lipids requires innovative in vitro and in vivo synthetic biology and chemical synthesis using novel catalysis to sustainably manufacture precision medicine products and supplements.

Specific challenges:

- Advanced processes to sustainably scale-up the production of specialty carbohydrates, glycans and lipids. This could be by combining synthetic biological methods, coupled with state-of-the-art chemical synthesis, including novel enzymes;
- Support cross-disciplinary research in academia and industry to develop and scale up the production of products at the quality standards required for safe alimentation and at affordable costs for the broader population by upscaling sustainable manufacturing research using bio-informatics, glycomics and metrology;
- Align microbiome studies with glycomics, lipidomics, metabolomics and other -omics (i.e., high-throughput tools to analyse carbohydrate and lipid profiles and function, establish open-access databases and generate new standards);
- Utilise recent studies on carbohydrates, glycans, and lipids in promoting a healthy microbiome to identify and validate biomarkers for novel health, medical and dietary treatments.

Specific expected impact: Production and metrology of specialty glycans and lipids have applications in personalised medicine, personal care products (especially skin, mouth), dietary supplements and health food ingredients, with an overall contribution towards improving human health.

IMPACT EXAMPLES:

Example 1: Establishing a uniform approach to metrology and/or measurement of carbohydrates and lipids for biopharmaceuticals, diagnosis of disease and precision medicine, food and personal care, able to identify the current state-of-the-art and future innovation and technological challenges in carbohydrate metrology.[219]

TRL(now) & TRL(2030): Specialty carbohydrate and SPM synthesis and production elements are currently at a low TRL (1-3). For examples at higher TRL, there is still the need to increase production/process efficiency. More fundamental research at TRL (1-5) would be on exploring new (bio)-catalysts for carbohydrates and glycan synthesis and modification, or on improving metrological capabilities coupled with databases covering a range of –omics, but especially lipidomics and metabolomics. Advances in metrology and bio-informatics range from TRL 1 – 6. For these, more demonstration activities at higher TRL (5-7) need to be achieved by 2030.

3.10.3.3 Novel products for sustainable agriculture, forestry and ocean harvesting

Context: The updated EU Bioeconomy strategy aims to enhance the sustainable sourcing of feedstock, but also sustainable production and recycling.[220] Circular economy is thereby also at the core of the new strategy. Examples of renewable feedstock includes vegetable oils, starch, algae, and lignocellulosic biomass. In addition to biopolymers, there are many unrealised niches such as new biomolecules, biocatalysts and bacterioplankton displaying huge genetic diversity. Valorising renewable feedstock by developing concomitantly new biotech processes could allow the discovery and manufacture of yet undiscovered biologics. The opportunities include new sustainable agricultural practices for good soil quality, sustainable crop-care, targeted low-dose fertilisers and pesticides, and data mining for new products and organisms using metagenomics and transcriptomics.

Specific challenges:

- Using biomolecules, sourced sustainably from land and sea, improve the functional and material properties of novel functional food and personal product ingredients;
- Using data mining of acquired metagenomic data of ocean environs, coupled with transcriptomics, identify novel biocatalysts and biomolecules for future manufacture of medical, food and health products;
- Using transcriptomics and formulation science, develop fertilisers that target directly the crops or insecticides that attack selectively pests using epigenetic technology;
- Develop functional crop-care by relating the deeper knowledge of the microbiome of plants and soil to the application of beneficial microorganisms or phages with fungicidal or insecticidal activity which can protect agricultural crops;
- Using metagenomic tools to assess and monitor soil health, develop new products to repair soil damage and then maintain soil health in a sustainable manner.

Specific expected impact: Enable the production of novel products with positive environmental health implications such as improving soil health.

IMPACT EXAMPLES:

Example 1: Development of the first patented smart microbiome-based platform to identify the soil microbiome from a sample, with a database of soil microbial profiles, to provide valuable data to farmers, enabling them to make intelligent and personalised decisions. The 'precision agriculture software' market is expected to reach €1 189 million at a CAGR of 14.03 % by 2022, with high expected impact on the agri-food industry.[221]

Example 2: Development of a bio-pesticides from a bacterial strain with a proved efficacy in different major pests, providing a bio-product for highly intensive and environmentally friendly agriculture.[222]

TRL(now) & TRL(2030): Process development of novel biologics is currently at a low TRL (1 – 3), although some cases are already at TRL 5 and above. More fundamental research could be applied to explore sustainable agriculture, forestry and ocean harvesting for feedstock valorisation. Advances in transcriptomics, phage displays and bioinformatics databases, for novel biocatalysts and biomolecules are at TRL 2-6. RD&I on new techniques at TRL 5-8 needs to be considered by 2030.

3.10.3.4 Advancing the application of IB for the sustainable production of bio-based polymers

Context: Bio-based polymers represent an important value chain for industrial biotechnology, referring to the use of renewable biomass as feedstock and often also to the production methods applied (biotech), therefore expanding the choice of feedstock. Biotechnological steps can be used across the production pipeline and the output is bio-based polymers and bio-based plastics that can be durable or biodegradable, for a wide range of applications incl. packaging, textiles, building & construction and consumer products.[223] There are two main categories of bio-based plastics: drop-ins for existing mass markets, analogues of fossil-based polymeric counterparts (e.g. polyethylene terephthalate (PET), polyethylene (PE), and polyamide (PA)), but also dedicated, novel structures (e.g. polyethylene furanoate (PEF), polyhydroxyalkanoates (PHAs) and polylactic acid (PLA)), with PLA being a notable exception regarding reaching a commercial status. For bio-based polymers to achieve economies of scale, further RD&I is needed for application- and market- driven bio-based polymers with targeted functionalities and properties.

Specific challenges:

- Cost competitiveness improvements, in particular for drop-ins;
- Improved biotech process optimisation for polymers production over biomass feedstock flexibility (composition variability);
- Robust biocatalyst design against upstream and downstream contaminants.

Specific expected impact: The annual growth rates for bio-based plastics in Europe is estimated at 12 % by 2030, reaching approximately €5.2 billion market value.[224] The aim is to improve the process scalability, reliability, environmental performance, and reduction of lifecycle costs for bio-based polymers produced by the means of IB. The end-result will aim to be novel or drop-in bio-based polymers as the creation of new value chains that can bring the products to the market.

IMPACT EXAMPLES:

Example 1: Development of PLA, able to compete with standard thermoplastic grades used in packaging applications (such as PET and PE), achieving 50 % less energy and producing 10 times less emissions in comparison to standard thermoplastics like PET and PP.[225]

Example 2: Development of a 100 % renewable Polyethylene Furanoate (PEF) through wood-based fructose for production of plastic bottles and all plastic packaging.[226]

TRL(now) & TRL(2030): The development of bio-based polymers (e.g. PET, PE, PA) is currently at a TRL 2-4, albeit some bio-based polymers (e.g. PHA, PLA) having achieved a relatively high TRL (5-7). Further R&DI actions for scalable and sustainable process development, valorising 2G-3G feedstock by biotechnological routes to produce bioplastics needs to be considered by 2030.

3.11 Waste Valorisation Process Technologies

Context: The tremendous growth in waste generation all over the world has quickly become one of the global challenges of today's economy. Municipal waste including plastic waste and biogenic waste present the opportunity to become an alternative feedstock. Several novel processes are being developed to transform waste into chemicals, fuels and materials that can be used in chemical processes in contrast to waste incineration and landfill. Waste valorisation also comprises, among others, the recovery of critical raw materials such as phosphorus, metals, rare earth elements.

Market, overall expected impact: In 2014, the EU produced 2.5 billion tons of waste.[227] In 2016, the EU used about 50 million t of plastics per year, of which 27 million t of waste was collected and 27 % was still sent to landfill, leading to a loss of valuable resources.[228] About 8.4 million t entered recycling facilities and 11.3 million t were treated for energy recovery. Waste of electrical and electronic equipment (WEEE) is also one of the fastest growing waste streams in Europe, with some 12.3 million t generated in the EU in 2016 (and 44.7 million t worldwide), and expected to grow.[229] Overall, 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.

Waste valorisation technologies address several **Horizon Europe (HEU) clusters and areas of intervention:** 'Advanced Materials' 4.4, 'Circular industries' 4.8, 'Low-carbon and clean industries' 4.9, 'Energy supply' 5.2,' Clean, safe and accessible transport and mobility' (5.7), 'Energy storage' (5.9), 'Biodiversity and natural resources' (6.2), 'Agriculture, forestry and rural areas' (6.3), 'Seas, oceans, inland waters' (6.4),'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) mainly by:

- **More sustainable production contributing to circularity of materials and improved environmental impact** through sustainable end-of-life management and utilisation of recovered materials over the extraction of virgin raw materials;
- **Recycling plastics waste**[230] in particular from packaging, multi-layer films, textiles, composites from wind turbines and vehicles;
- **Recovering critical raw materials** (phosphorus, metals, rare earth elements) mainly from electronic waste and wastewater.

Horizontal challenges:

- Waste composition complexity, variation over time, access to homogeneous waste through improved upstream collection, logistics, sorting, separation, and pre-treatment;
- Removal of impurities such as colourants and additives, including hazardous substances, causing issues with the waste valorisation processes;
- Physicochemical and mechanical characteristics of recyclates compared to virgin materials;
- Control of degradation by-products upon recycling;
- Reducing energy intensity (and related CO_2 emissions of recycling processes) through process optimisation.

SUSCHEM PILLARS – MULTI-KETS:

Waste valorisation processes will enable and will be enabled by the circularity-by-design highlighted in the **Advanced Materials section (Chapter 2)** in particular for: 'Composites and cellular materials (2.1)', 'Bio-based chemicals and materials (2.3)', 'Additives (2.4)', 'Membranes (2.7)', 'Materials for energy storage (2.8)' and 'Coating materials and aerogels (2.9)'.

Enabling Digital Technologies (Chapter 4): 'From coordination and management of process/plant/site to connected value chains towards industrial symbiosis 4.3', 'Process Analytical Technologies (PAT) 4.4', 'Data sharing platforms / data security 4.8', 'Distributed-ledger technologies 4.9' and 'Enabling transparent supply chains (4.9.1)'.

Within **Advanced Processes** the relevant topics include: 'Tolerant and Intensified Reactors and Processes – tolerance to feedstock variability (3.1.1)', 'Membrane reactors - integrated systems (3.1.6)', 'Modular production (3.2)', 'Separation process technologies (3.3)', 'New reactor and process design using non-conventional energy forms (3.4)', 'Electrochemical processes for waste treatment to recover valuable materials including catalysts (3.5.2)', 'Enhancing biomass catalytic valorisation (3.9.1)', 'Enabling waste valorisation via catalysis (3.9.2)', 'Industrial Biotechnology 3.10' and 'Process technologies for advanced water management 3.12'.

RD&I Actions

3.11.1 Chemical recycling of plastics waste

Context: Plastics waste recovery and treatment is recognised as a priority at European level. Evidence for this is the European Strategy for plastics in a circular economy, which aims at making plastic packaging recyclable by 2030.[231] However, plastics waste is one of the most complex material mixtures from a recycling perspective. The recycling effort includes various methods, such as pyrolysis, gasification, depolymerisation, or biotechnological processes.

IMPACT EXAMPLES:

Example 1: Treating plastic waste including end-of-life composites and non-recyclable packaging waste to produce valuable chemicals (alkylaromatics) via a multi-step process comprising of pyrolysis and sequential catalysed reactions and separation steps, able to reduce CO_2 emissions by 40-55 %, residues up to 95 % and energy use by 45 %.[232]

Example 2: Improve the separation and recycling of urban bulky waste - implementing advanced fragmentation techniques (e.g. gasification) - to obtain high value chemicals or fuels.[233]

Example 3: Avoiding the landfilling of textile waste from the footwear industry and recycling it chemically by means of catalytic glycolysis (solvolysis), achieving a GHG emissions reduction estimated around 1.47 t CO_2 eq /t PET produced.[234]

Example 4: Process intensification of chemical recycling of PET waste through microwave assisted catalysed solvolysis, addressing the difficulty of plastic packaging management. More than 1 million tons per year could be treated with this technology.[235]

Example 5: Mechanical sorting and chemical recycling of 'residual textile waste' (unwearable/ unusable textile waste that is disposed via landfill or incineration in the absence of other valorisation routes today) to produce alternative fuels and wood panels adhesives.[236]

Example 6: Plastic depolymerisation process through solvolysis together with an enzyme catalyst, followed by re-polymerisation to PHA using engineered microorganisms.[237]

TRL(now) & TRL(2030): Pyrolysis technologies are currently at TRL 3-5 with a range of maturities that go from concept all the way to small demo plants depending if waste-to-fuel or waste-to-chemicals is considered. Gasification processes, which can possibly be combined with biological and chemical post-treatment, show a wide TRL range while currently pilot and demo plants are under investigation. The waste-to-monomers through solvolysis is relatively well developed for some types of polymers (TRL 3-5), for instance for polyethylene terephthalate (PET) and polystyrene (PS) but lacking behind for polyolefins. Biotechnological processes for plastic waste valorisation are currently at TRL 2-3. More fundamental research is thus needed to reach a TRL 5 by 2030.

3.11.1a. Chemical recycling of plastics waste by pyrolysis

Context: Pyrolysis is conducted at high temperatures and in the absence of oxygen; it is particularly applicable to mixed polymer waste. 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. Lower temperatures applied during the catalytic process yield faster degradation and a narrower fractional composition of the products.

Specific challenges:

- High energy-intensity required due to high process temperatures;
- Prevention and/or removal of hazardous and corrosive compounds that can be generated during the process add into process complexity, scalability and safety challenges;
- Reactor fouling due to by-products (ash);
- Dehalogenation procedures are necessary, because the oils collected in single pyrolysis process may contain numerous halogenated organic compounds, which would detrimentally impact the reuse of pyrolysis oils.

3.11.1b. Chemical recycling of plastics waste by gasification

Context: 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 H_2 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 utilised to moderate temperatures in the process and to increase the yield of H_2. Gasification has the potential to be applied where waste cannot be treated neither by mechanical recycling nor by pyrolysis.

Specific challenges:

- Feeding system of waste material at high-pressure gasification, in a continuous process;
- High temperature/energy requirements;
- Fouling due to by-products (ash and particles);
- Tars, heavy metals, halogens and alkaline compounds can be released within the product gas, causing environmental and operational problems for the gasification of some waste streams;
- Process flexibility to cope with short-term and/or long-term variation of waste feedstock composition.

3.11.1c Chemical recycling of plastics waste by depolymerisation: solvolysis

Context: Depolymerisation, as a conversion 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. In solvolysis, certain polar and semipolar solvents (e.g. water: alcohol; glycol) are excellent reaction media for depolymerisation of plastics. 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, and textile polyesters.
Solvolysis can also be seen as pre-treatment for separation in polymer waste streams due to its high chemical selectivity. For composites, depolymerisation also allows the recovery of fibres and fillers.
In addition, circularity-by-design is expected to facilitate plastic waste treatment by depolymerisation.

Specific challenges:

- Ensure constant input specification of End-of-Life (EoL) material;
- Critical pre-treatment step of input material;
- Robustness of process to deal with the potentially high content of impurities of EoL materials;
- Batch to continuous to improve competitiveness at commercial scale;
- Downstream separation and purification of individual monomers after depolymerisation (as trace solvents and other contaminants influence the reprocessing);
- Large volume of solvent and significant energy is required for solvent recovery.

Only a limited number of EoL polymers exist in a sizable amount that can be converted via depolymerisation, since one of the main issues is the accessibility of suitable EoL materials (preferably mono-streams). Beside the process optimisation, collection systems and sorting technologies are essential to access easy-to-process waste.

3.11.1d. Biotechnological processes, applying microbes and enzymes for plastic recycling

Context: Plastic waste can also be treated using microorganisms and enzyme catalysts that can be potentially engineered to adapt at the required conditions (see Advanced processes: Industrial Biotechnology 3.10). Enzymes have already been identified to modify and/or break down various polymers; further engineering approaches are developed for catalytic activity enhancements.[238] Biotechnological technologies could enable recycling at much lower energy-intensity, thereby potentially reducing process-related CO_2 emissions. However, it is critical to prove the scalability of such solutions.

Specific challenges:

- Identification and engineering of range of enzymes and microorganisms that can be applied on bulk production polymers with variable physicochemical properties;
- Cost competitiveness and scale up (key upstream and downstream purification issues).

3.11.2 Chemical valorisation of secondary biomass sources

Context: Biomass, including second generation non-edible sources, forestry and agricultural residues, has been extensively studied as a potentially abundant feedstock. The benefits of processing residual biomass could extend from feedstock diversification to new business models and growth in rural areas. However, the viability of integrated biorefineries is critically impacted by the technological readiness of highly efficient and sustainable processes for a range of products, across existing and new value chains. The technology development of bio-based products can be based on chemical, thermo-chemical routes and/or biotechnological routes.

The valorisation challenges and opportunities of lignocellulosic and non-lignocellulosic feedstock are further elaborated under 'Bio-based chemicals and materials (2.3)', 'Advancing the application of IB for the sustainable production of bio-based polymers (**3.10.3.4**)', but also under 'Enhancing biomass catalytic valorisation (**3.9.1**)'.
With regards to waste biomass pre-treatment and thermochemical processing, similarities of context and

challenges could be found under section **3.11.1** which is dedicated to the chemical valorisation of plastics waste.

3.11.3 Critical raw materials recovery from waste

3.11.3a. Phosphorus and other primary elements recovery

Context: Phosphorus is a key nutrient with crucial importance for agriculture and global food security. For instance, the annual demand for phosphorus is rising nearly twice as fast as the growth of the human population.[239] Phosphate rock is an intensively exploited finite resource, concentrated in a few countries worldwide, leading to strong import dependency and insecurity due to resource deficits. In 2017, the European Commission declared phosphate rock and phosphorus within the 27 critical resources for the EU. Significant efforts and priority funding were focused on developing materials and technologies for phosphorus recovery from secondary sources, such as sewage sludge from wastewater treatments. The vast majority of phosphorus is used in fertilisers, with other applications in organophosphorus compounds in detergents, pesticides, insecticides, food additives, production of ceramics, pharmaceutical and cosmetic excipients and isotopic tracers among others.

Specific challenge:
Optimise separation processes to improve the efficiency of phosphate recovery from biomass digestates, sewage sludge, municipal and/or industrial wastewater.

3.11.3b. Scarce metals and resources recovery from electric and electronic waste

Context: Increasing technological development is driving the demand for metals, especially in the field of electronics. Conversely, electric, electronic and batteries waste is a growing global waste stream, highly problematic in its management. Unsafe disposal contributes to pollution as well as wasting resources, causing human and environmental health risks. Metal concentrations in electronic waste are often higher than in mineral ores and some metals are considered critical in supply, thus this is a strong incentive to recover them from an alternative source. The recovery of valuable metals from electronic waste can be achieved with physical, chemical, biological methods or combinations thereof. Bioleaching, involving microorganisms, is working at near ambient temperatures, with positive environmental performance attributes for metal recovery processes. Emerging technologies include alternative solvents, such as ionic liquids, and electrochemical processes.

Specific challenges:

- Improvements in technologies to prevent significant losses of valuable elements;
- Improvements on reactor design for scale-up for bioleaching and electrochemical processes;
- The current continuous bioleaching operations are also being challenged by the presence of hydrocarbons in the bioreactors. These compounds may enter the production chain and inhibit bacterial activity; [240]
- For alternative solvents, such as ionic liquids, mass transfer and cost of scale-up can be challenging, requiring finetuning of structure and physicochemical properties.

IMPACT EXAMPLES:

Example 1: Development of a novel technology able to recover 113,000 t/y of P in municipal sewage water, estimated to cover 26 % of the mineral P-demand in North West Europe.[241]

Example 2: 90 % waste recovery from permanent magnets and secondary batteries waste, 50 % energy savings, and recycling and reuse of the ionic liquid through a novel technology based on recently developed lab-proven technologies for direct high-temperature electrolyses of Rare Earth Alloys (REA) production.[242]

Example 3: 98.4 % copper removed from electronic waste by bioleaching, a biologically mediated natural chemical process.[243]

TRL(now) & TRL(2030): Technologies of P-recovery from wet sewage sludge and sewage sludge ash are currently at TRL 6 but rather fragmented across countries due to wide differences in waste regulatory measures and actions. Demonstration activities for homogeneous market uptake and recovery plants distributed in all countries need to be considered by 2030. Standard technologies of metal recovery have achieved a TRL of 6-7 while bioleaching is at TRL 3-4. Thus, demonstration activities are needed for the later technique to reach TRL 7-8 by 2030.

See also*: *'Electrochemical processes for recovering valuable materials, including catalyst'* (3.5.2**) *and 'Separation process technologies' (3.3)*

3.12 Process Technologies for Advanced Water Management

Context: Water is a resource coming under increasing pressure due to a growing world population, climate change and an intensified industrial activity. It is estimated that water scarcity affects more than 40 % of the global population and 80 % of wastewater from human activities is discharged into waterways.[244] It is imperative to develop inexpensive, scalable and sustainable processes and methods for water treatment/water management to sustain a healthy planet and ensure clean drinking water. Moreover, water reuse and recycling ('zero liquid discharge') and water symbiosis are key topics for the process industries, including the chemical sector. The development of membranes for water separation and treatment is key together with enabling digital technologies, such as sensing technologies (PAT), that contribute to smarter water systems by implementing real-time online data. Advanced (big-) data analytics and artificial intelligence will support water operations decision making, risk management, control and use.

Market, overall expected impact: The development of materials and processes for water treatment, complemented by digital tools, contribute to reduced costs and energy input requirements to improve the overall efficiency of water treatment processes, whilst protecting human and environmental health.

Process technologies for advanced water management address several **Horizon Europe (HEU) clusters and areas of intervention**: 'Circular industries' 4.8, 'Low-carbon and clean industries' 4.9, 'Biodiversity and natural resources' (6.2), 'Agriculture, forestry and rural areas' (6.3), 'Seas, oceans, inland waters' (6.4), 'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) mainly by:

- **Improved resource and energy efficiency** in water treatment processes;
- **Water treatment and seawater desalination** at lower energy;
- **Water symbiosis and closing the water loop;**
- **Improved water quality to enhance positively human and environmental health.**

Horizontal challenges:

- Developing novel and more energy efficient water treatment processes through combined materials and process innovation;
- Developing new digital tools that can be used for the control of water treatment.

SUSCHEM PILLARS – MULTI-KETS:

Process technologies for advanced water management will be enabled by **Advanced Materials (Chapter 2)** in particular 'Membranes (2.7)'.

Relevant **Enabling Digital Technologies (Chapter 4)** include: 'Coordination and management of connected processes at different levels 4.8'; 'Process Analytical Technologies (PAT) 4.2', 'Data sharing platforms and data security 4.7' and 'Advanced (big-) data analytics and artificial intelligence 4.4'.

Within **Advanced Processes** the relevant topics include: 'Modular production (3.2)', 'Separation process technologies (3.3)', 'Industrial Biotechnology 3.10' and 'Electrochemical processes for recovering valuable materials, including catalyst (3.5.2)'.

RD&I Actions

3.12.1 Water reuse and recycling - Closing the water loop ('zero liquid discharge')

Context: Process industries are facing increasing water stress, e.g. more than 40,000 million m3 of waste water is treated in EU every year, but only 964 million m3 of this treated wastewater is reused.[245] Main drivers for an increasing water stress are climate change and competing water demands from industrial, public and agricultural water users. An integrated industrial water management, fostering recovery, 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.

Specific challenges:

- Enabling water conservation, reuse, recycling, by addressing industry process water flows, with the objective to reduce water footprint in an economically and ecologically (e.g. energy and CO_2) efficient way;
- Production process development and scale-up in combination with water treatment technologies to enable water reuse and target full closure for industrial water loops;

- Development and scale-up of extraction/separation technologies to enable extraction and valorisation of components from water reuse residue streams;
- Valorisation of low temperature (< 50 °C) waste heat from wastewater and water reuse streams.

Specific expected impact: 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.

IMPACT EXAMPLES:

Example 1: OPEX was reduced by up to 30 % for every m^3 of saved freshwater/year; eliminating the need for incineration (e.g. 5 000 tonnes/annum/plant) together with establishing a business case, leading to revenue generation; reduced fresh water uptake of 40 – 80 % resulting in freshwater savings of ~3 million m^3/year in one case; reduced wastewater production of 30-80 %, with close to 100 % (loop-closure) in one case and resulting in reduction of wastewater production by ~2.5 million m^3/year in another case; efficiently extracting resources from water and returning these to the prime process or a local increase in resource efficiency by use of algae; reduced energy use of up to 20 % by using low-energy technology, heat recovery, or optimising the integrated process with the use of improved modelling.[246]

Example 2: A flexible system for water management in industries that can be integrated to existing systems. Technological innovation included a holistic solution in the area of selected membrane technologies, a strong field magnetic particle separator, and a catalyst to prevent biofouling, including valorisation of waste heat. The impact is linked to increasing process water efficiency as well as resource, water and energy savings in the process industry (increase water and resource efficiency by 20-30%).

TRL(now) & TRL(2030): Technology and management schemes close to a full water loop closure and first approaches for residue valorisation have achieved a TRL 5, more R&I on demonstration and optimisation at TRL 6-8 need to be considered by 2030. More fundamental research at lower TRLs (1-5) is needed on routes forward to connect production process development and scale-up with accompanying water treatment schemes and for the valorisation of low temperature waste heat, towards reaching a TRL of 5-6 by 2030.

3.12.2 Alternative water sources and Water Symbiosis

Context: Fostering water efficiency in process industry and independence from freshwater resources, beyond on-site water recycling and reuse, requires an enhanced integration perspective of industrial water management. 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).

Specific challenges:

- Establish procedures to ensure compliance with required specifications and criteria;
- Overcome regulatory limitations to enable circular/ symbiotic approaches and the use of waste water as a resource.

3.12.3 Decentralised/smaller treatment systems

Context: Specific, separated streams of used water (e.g. wastewater of specific processes, washing water from plant cleaning) can be treated effectively at the source. 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.

Specific challenges:

- Cost efficient, robust and reliable sensors and analytical tools for a wide range of parameters, operable in an online and real-time environment are needed to allow an appropriate control and management of decentralised systems;
- Modular treatment systems are needed to operate decentralised systems in a flexible way, adapted to dynamics and increasing flexibility in industrial production.

3.12.4 PAT – water operations and treatment

Context: 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.

Specific challenges:

Sensor development for new parameters affecting:

- Process control (e.g. genre probes for biological wastewater treatment);
- Plant availability (e.g. corrosion, scaling, fouling);
- Quality control (e.g. micro pollutants, microorganisms, algae).

Sensor development to extend application.

Sensors for online and real-time monitoring of parameters, enabling:

- Self-calibration, auto-adaptation and (self) learning;
- Process and plant control to provide maintenance-relevant data for predictive maintenance;
- Creation of sensor networks to control water systems and to collect operation relevant data for a dynamic operation of (waste)water treatment systems.

Sensor development to decrease cost and increase robustness.

Sensors for comprehensive networks and demanding requirements providing:

- High-quality data, (close to) real time while being in a (low) cost range that allows a sufficient equipment of water management systems;
- Low maintenance requirements (e.g. plug and operate, self-calibration) and high sensor reliability (e.g. in demanding environments: fouling, corrosion, abrasion) for a long service life;
- Energy efficient operation.

Specific expected impact: In the industrial water management context, new sensor developments will provide reliable data sets that are necessary to make use of digital data processing tools e.g. advanced data analytics and Artificial Intelligence (AI). In addition, they will provide the basis for digital process twins in industrial water management. New sensor developments will also contribute to improved operation times of water treatment systems and thus foster efficiency and safety in operation.

**For Impact examples and TRL, please see 'Process Analytical Technologies (PAT)' 4.2.*

3.12.5 Water data management [Advanced data analytics & AI]

Context: Enabling industrial water management with digital technologies, under an 'industrial water 4.0' context, and connecting it with industrial production, municipal (waste) water management and water resource management is generating comprehensive data sets (big data). These data provide the basis for enhanced decision support, governance and management systems. To convert data into information suitable for decision making and management, advanced tools for data analysis and data management are needed. Artificial Intelligence (AI) can be of help for comprehensive and complex data sets. Especially at the interface between production and water management, a fast, reliable and efficient data management is indispensable for a resource efficient integrated industrial water management.

Specific challenges:

- Flexible algorithms are needed for data analysis to support water operation decision making, risk management, model development and use considerations on integrated system level;
- To valorise big data and IoT information (e.g. control systems for water networks), advanced technologies and capabilities (e.g. HPC –high performance computing) for quasi-real time data analysis, forecasting, visualisation and communication are needed for advanced decision support and management;
- Development of digital process twins for industrial water management, connected with process control and manufacturing execution systems;
- Water data security, open format standards and trust in sharing data are needed to be able to share data across industries and to merge data from private and public sectors.

Specific expected impact: An advanced, digitally-enabled, 'smart' industrial water management will foster the industrial water value chain and its connection with other water users and water resources management stakeholders. It will support efficiency and reliability along the production value chain in process industries.

**For Impact examples and TRLs, please see 'Advanced (big-) data analytics and artificial intelligence' 4.4.*

4 ENABLING DIGITAL TECHNOLOGIES

SUSCHEM

Digitalisation Transforms the Chemical Industry Rapidly Across its Entire Value Chain

ADVANCED MATERIALS

ADVANCED PROCESSES

ADVANCED PROCESSES

Management of feedstock supply

Big data-driven raw material analytics to optimize feedstock costs, flexibilisation in feedstock (including waste, biomass and CO_2)

R&D/ Laboratory 4.0

Machine-learning and artificial intelligence-driven research, advanced materials and formulation simulation, digital process development, digital twins, laboratory automation and high throughput screening

Cognitive plants

PAT-based real-time model predictive control and process optimisation based on physical properties models enhanced by advanced data analytics/AI

Supply chain integration

Production data sharing with suppliers/real-time supply tracking, digital tools enabling more efficient procurement processes

New forms for collaboration & co-creation

Platforms for exchanging R&D data, platforms to collaborate and for data exchange, co-creation within the sector and beyond

Process analytics (PAT)

Advanced sensing and process-analytical technology for tighter closed-loop process monitoring and control, at reasonable cost

ADVANCED PROCESSES

SUSCHEM ENABLING DIGITAL TECHNOLOGIES
DIGITAL INNOVATIONS FOR THE CHEMICAL INDUSTRY

ADVANCED MATERIALS

Predictive maintenance

Advanced analytics-based predictive and risk-based asset maintenance

Management of processes

Scheduling of connected processes within plants and sites

Supply chains in a circular economy

Increase transparency through tracking and tracing of products throughout life-cycles, e.g. by blockchain technology

New roads-to-market

Digitalisation of customer experiences, involving customers and/or consumers into the product development cycle, providing additional services, disruptive new business models

Risk management

Advanced analytics-based cybersecurity management

Industrial symbiosis

Model-based coordination and management of energy and material flows across industries and with municipalities/cities

Operator support

Advanced process interfaces, augmented reality, digital twins for training purposes

SUSCHEM ENABLING DIGITAL TECHNOLOGIES
DIGITAL INNOVATIONS FOR THE CHEMICAL INDUSTRY

Digitalisation will be a source and driver of transformational change across the chemical industry, with an emphasis on safety, operational excellence and sustainability. The change will happen horizontally and cover the entire life cycle, including R&D, operations for production, supply chain and sales processes, across the entire value chain and across industry sectors. Digital technologies have the potential to reduce CO_2 emissions by 60-100 million tonnes and avoid 2,000 to 3,000 injuries over the next decade.[247] The transformation of the chemical sector requires the blending of digital and physical 'worlds', central to the new global wave of innovation. Digital transformation is a major driver, enabling innovation in Advanced Materials (**Chapter 2**) and Advanced Processes (**Chapter 3**).

Digital Key Enabling Technologies applied within product, process development and engineering stages will largely speed-up innovation and the experimental design phase, allowing a more efficient "idea-to-market" process. Data-driven innovation in the chemical industry of the future combines inputs from sensors, data from products and raw materials, data from marketing and sales, and other available information. These inputs are analysed by advanced Artificial Intelligence (AI) and Machine Learning (ML) technologies with a massive impact in multiple areas: production, regulation, safety, supply chain and logistics, among others. Digitalisation will allow to quickly respond to market demands through integration of customers into the R&D-process. It will allow engineering and plant operation in an integrated way along the whole lifecycle of a plant, starting from process development, engineering, procurement, construction, commissioning, operation to plant flexibility and potential retrofit.

New digitally-enabled solutions improve process control and operations efficiency and reliability. These new solutions will further optimise the processes themselves, e.g. through sensors, model-based control and predictive maintenance. They will also significantly improve production management by considering product quality, energy and resource efficiency of connected processes and plants. Digitalisation of manufacturing and plant operations will be disruptive by significantly reducing manual work and allowing for the efficient free flow of information for improved decision making by operators. Allowing for upstream and downstream secure information sharing could also significantly impact product quality and process efficiency.

Digitalisation will also change today's supply chains by enabling multiple connections through data across both upstream/downstream parts and other industrial sectors, achieving more economically and environmentally efficient operations, e.g. through production management of connected plants and chemical sites towards industrial symbiosis. The chemical industry will develop new data and service-based business models, simultaneously, products will increasingly incorporate digital service components, enabled by big data, to strengthen the competitiveness of the entire offer.

The relevance of distributed-ledger technologies in business capabilities becomes applicable in areas such as transparency of supply chains. In the context of transitioning to circular supply chains, such technologies enable tracking of materials and products along lifecycles.

Summary of key priorities for enabling digital technologies to be addressed:

- Increase the impact of novel digital technologies into **R&D, process development** and **plant engineering processes**;
- Apply **Digital Twins** (combining first principle models, data-driven models, semantic models) for the whole process and product lifecycles;
- **Advanced sensing** and **process-analytical technology (PAT)** for closed-loop process monitoring and control, including multi-sensor data fusion and including plant retrofitting;
- **Cognitive plants** - apply **advanced data analytics, AI and model predictive control**, in combination with other model-based technologies, including for predictive maintenance and **self-organization of production**;
- Addressing the **quality and reliability of data** including storing of data (e.g. **data sharing platforms**) and aspects **of cybersecurity** (e.g. save process operation);
- Integrated **production management of plants and chemical sites/parks** for optimised sustainability and agility, such as integration with the electricity grid (demand-site response) and **industrial symbiosis**;
- Digitalisation of **whole value chains** including dataflows and aspects of logistics including feedback from customers and circular economy aspects, using **distributed ledger technologies** to track throughout value chains;
- New forms of **collaboration of humans/operators** with advanced control and optimisation systems, through digital operators' support.

Priorities such as advanced data analytics, AI, data sharing platforms, cybersecurity, distributed ledger technologies would require strengthening the reach of the chemical industry into the digital sector. On the other hand, the well-established know-how of the chemical sector on R&D, process design, process automation and control imply its leadership in innovation initiatives to implement the full potential of digital transformation.

Impact of enabling digital technologies – UN SDGs

'Industry Innovation and Infrastructure', with the full set of digital technologies, applicable to the chemical sector, enabling the development of reliable, sustainable and resilient infrastructure for sustainable industrialisation in addition to retrofitting industries to increase resource efficiency and the greater adoption of clean and environmentally sound technologies;

'Responsible consumption and production' by facilitating the design of circular materials, the tracking of products throughout value chains, towards recycling and reuse, as well as industrial symbiosis to reduce waste and therefore optimise energy and resource efficiency;

'Climate action', through digitally enabled processes that can be applied for greater energy efficiency to lower GHGs emissions;

'Clean water and sanitation', supporting water data management and sensors to improve water usage;

'Affordable and Clean Energy', via the integration of renewable energy into production, through digital tools for demand-site management;

'Decent work and Economic Growth' via automation to establish more productive and safer working environments, but also through technological upgrading, innovation and faster scale-up.

Enabling Digital Technologies innovation – relevance to Horizon Europe and Digital Europe

Digital technologies innovation presents a major contribution to the long-term European policy goals and national digital initiatives. To address these key priorities for digital technologies within the chemical sector, a co-creation innovation process will be crucial, amongst sectors but also along the innovation ecosystem. The need for a close collaboration with highly innovative deep tech start-ups is highlighted, with contributions from Academia and Industry, thereby linking with HEU Pillar 3 ('Innovative Europe'), Pillar 1 ('Excellent Science'), and Pillar 2 ('Global challenges and European industrial competitiveness'), respectively. Given the thematic approach of Pillar 2, the high relevance on the Horizon Europe clusters and areas of intervention is further elaborated (Table 6).

Innovation in digital technologies should deploy different instruments, and initiatives in a system integrated way, seamlessly over the boundaries of different funding mechanisms, beyond Horizon Europe. The **Digital Europe Programme** is expected to bring additional value for building essential digital capacities, and accelerating the best use of technologies, in the chemical sector especially AI, distributed ledger technologies, Big Data, cybersecurity and advanced digital skills.

Table 6: Relevance of SusChem Priorities on Enabling Digital Technologies with Horizon Europe

Horizon Europe

Pillar 2: Global Challenges and European Industrial Competitiveness

Clusters and Intervention areas

CLUSTER 1: Health	1.1 Health throughout the life course
	1.2 Environmental and social health determinants
	1.3 Non-communicable and rare diseases
	1.4 Infectious Diseases, including poverty-related and neglected diseases
	1.5 Tools, technologies, and Digital solutions for health & care, including personalised Medicine
	1.6 Healthcare systems
CLUSTER 3: Civil security for Society	3.1 Disaster-resilient society
	3.2 Protection and security
	3.3 Cybersecurity
CLUSTER 4: Digital, Industry and Space	4.1 Manufacturing technologies
	4.2 Key Digital technologies
	4.3 Emerging enabling technologies
	4.4 Advanced Materials
	4.5 AI and Robotics
	4.6 Next generation internet
	4.7 Advanced Computing and Big Data
	4.8 Circular Industries
	4.9 Low-carbon and Clean Industries
	4.10 Space including Earth observation
CLUSTER 5: Climate, Energy and Mobility	5.1 Climate Science and solutions
	5.2 Energy supply
	5.3 Energy grids
	5.4 Buildings and Industrial facilities in Energy transition
	5.5 Communities and cities
	5.6 Industrial competitiveness in transport
	5.7 Clean, safe and accessible transport and mobility
	5.8 Smart mobility
	5.9 Energy storage
CLUSTER 6: Food, Bioeconomy, Natural Resources, Agriculture and the Environment	6.1 Environmental Observation
	6.2 Biodiversity and natural resources
	6.3 Agriculture, Forestry and rural areas
	6.4 Seas, Oceans and inland waters
	6.5 Food systems
	6.6 Bio-based innovation systems in the EU Bioeconomy
	6.7 Circular Systems

SusChem priorities: ENABLING DIGITAL TECHNOLOGIES

Laboratory 4.0-Digital R&D	Cognitive plants (real-time) process simulation, monitoring, control, optimisation	Process analytical technologies (PAT)	Advanced (big-) data analytics/artificial intelligence	Predictive maintenance	Data sharing platforms/data security	Distributed-ledger technologies	Digital support of operators and human- process interfaces	Coordination and management of connected processes at different levels
			●		●			
	●		●		●			
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●		●
●	●	●	●	●	●	●	●	●
	●	●		●	●	●		●
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●	●	●
			●		●			
●	●	●	●	●	●	●	●	●
					●	●		●
		●	●		●			●
					●	●		
●	●	●	●	●	●	●	●	●
●	●	●	●	●	●	●	●	●

4.1 Laboratory 4.0 – Digital R&D

Context: R&D laboratory 4.0 brings digital technologies into the research laboratory, automating the capture and flow of data from all the networked instruments and systems within the lab and beyond. Digitalisation will allow a quick response to market demands through integration of customers into the R&D-processes. Digitalisation will enable the ability to integrate life-cycle assessment towards the targeted solutions. Digital R&D technologies improve all steps of the R&D-cycle: Ideation, experimentation and automation. Digital R&D technologies in the chemical industry encompass, among others, modelling of chemical processes (e.g. reactor design, process design) but also materials and formulations design. Moreover, to optimise R&D-workflows, artificial intelligence is coupled with the R&D-data management from multiple sources and includes high-throughput screening, robots for laboratory experimentation, and augmented reality to support technicians and scientists.

Market, overall expected impact: Chemical companies that have implemented digital R&D show improvements from 20-50 % in their overall performance (20-40 % more projects, 20-40 % higher success rate, 30-50 % higher revenue, 30-40 % lower costs, 20-40 % lower time-to-market).[248] R&D laboratory 4.0 thus contributes to reduced costs, greater efficiency, more reproducible results, faster scale-up and improved collaborations; whilst enhancing workforce capabilities and further improving health and safety.

Digital R&D technologies address several **Horizon Europe (HEU) clusters and areas of intervention areas:** 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and Industrial facilities in energy transition' (5.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7) and 'Cybersecurity' (3.3), mainly by the following factors:

- **Reduced costs and improved efficiency** by applying digital R&D within early product/process design and development stages, which speed-up innovation and allow a more efficient "idea-to-market" process, including leveraging earlier experimental data/company knowledge in the experimental design phase;
- **Improved reproducibility of results** by applying digital R&D to analyse large volumes of data, increase the speed to scale-up due to the capacity to experiment faster and in an accurate manner, whilst enhancing the capacity to handle more complex data and multi-parametric experiments. This is of crucial importance, considering the complexity of the chemical industry, and increasing with circular economy (e.g. recycling-by-design, new variable composition of feedstock etc.);
- **Improved collaborations** especially **interdisciplinary** and **cross-sectorial**, through digital R&D, which will also allow a quick response to market demands through integration of customers and value chains into the R&D-process;
- **Digital platforms will enable research collaborations across the full innovation ecosystem:** SMEs, start-ups, Academia, and the process industry.

Horizontal challenges:

- Integrating more connected tools, able to be gathered into modular and evolving platforms;
- Creating and managing the ecosystem of digital tools and databases across complex R&D pipelines;
- Developing engineering methods and tools that build on existing data and know-how to be able to advance data analytics;
- While the volume of data constitutes a challenge, the big challenge is in the variety of forms of data, and its veracity;
- Increasing transfer of knowledge by means of algorithms and AI-based systems;
- Accelerating a sustainable circular economy by integrating topics such as safe-by-design, sustainability assessment, circularity-by-design, feedstock complexity to be tackled already at R&D design and experimentation stage and in early steps of supply chains;
- Access and exchange of data is a prerequisite, thereby a challenge is data confidentiality (e.g. privacy, regulations, IP-protection).

SUSCHEM PILLARS – MULTI-KETS:

Digital R& D is expected to have a strong horizontal impact on RD&I in Advanced Materials (Chapter 2) and Advanced Process technologies (Chapter 3), especially at lab-stage research and for technologies at low TRLs.

Within **Enabling Digital Technologies**, the relevant topics include: 'Advanced data analytics and Artificial intelligence 4.4', 'Digital support of operators and human-process interfaces 4.6' and 'Data sharing platforms, data security 4.7'.

RD&I Actions

4.1.1 Materials and molecules design: modelling and simulation developments

Context: Digital technologies can be used for the design and optimisation of functional materials (incl. composites, 3D-printing, bio-based materials and chemicals, complex formulations, catalysts). In the chemical industry, R&D cycles start with a given application profile, followed by complementing it with existing knowledge (literature, patents, proprietary data), modelling and simulation, design of experiments, experiments, analytics, and data analysis. With its main goal of making R&D more efficient and effective, materials modelling has become an essential part of this R&D cycle. Using molecular modelling, physical and chemical phenomena of systems can be quantitatively described using mathematical equations or algorithms, allowing for tailored performance characteristics and meeting application-specific challenges.[249] Applications of material modelling range from highly accurate predictions at atomic to system levels, such as polymers. It is used in diverse areas, e.g. complex formulations such as in home/personal care, coatings, crop protection) and properties of organic and inorganic materials (e.g. solid-state properties, chemical stability). High-performance computation and simulation have allowed to calculate - in short time - a large set of novel complex molecular structures (e.g. polymers or bio-molecules) and their behaviour in applications, opening completely new possibilities which were impossible due to the previous lack of computing power and cost.

Key specific challenges:

- Data-driven approaches have made significant progress and have proven to be widely applicable: e.g. machine learning to learn features of molecular or physics-based models. These surrogate models are much cheaper to compute compared to traditional multi-scale models and enable virtual screening of new materials in an unprecedented manner; hence more development is needed;
- Training of empirical models with experimental data. Novel approaches include adversarial models generating new data to overcome common limitations of empirical models;
- Use high performance computing to improve on materials design, based on physical principle models. Hybrid models that would also involve data-driven approaches is also needed;
- Design and simulation agility to adapt to circular economy and bio-economy (feedstock variability), i.e. bio-based materials may present higher property fluctuations across batches;
- Integration of complex parameters (as properties) of topics like safe-by-design, sustainability, circularity-by-design, and feedstock complexity/variability in materials design and simulation.

Specific expected impact: Materials modelling to achieve significant impact on reducing R& D costs, and accelerating time-to market but also increasing safety at work. These improvements in material modelling will thus bring the industry closer to modelling real systems and closer to production and customer needs.

IMPACT EXAMPLES:

Example 1: Developing an open web-based platform to collect, adapt and integrate all scattered modelling components from all fragmented materials modelling and industrial communities and provide a single point of access - an online gateway - to all materials modelling activities in Europe, strengthening the competitiveness and lowering the innovation barrier for the European industry for product development and optimisation using materials modelling.[250]

Example 2: Application of quantum chemistry by establishing a GPU-optimised Gauss based, efficient, parallel quantum chemical integrator module able to develop medicine molecules by replacing difficult and expensive tests with simulation techniques. This can significantly reduce the required time of the market launch, helping chemists find the perfect candidate with the perfect features and reducing the chance of molecules failing during further phases of the development. [251]

TRL(now) & TRL(2030): R&D digital technologies used for modelling materials have achieved a relatively low TRL (1-5), thus more research would be on exploring new R&D digital technologies that enhance materials modelling, or new methods for developing better algorithms. Some R&D digital technologies related to the use of digital imaging for modelling materials have achieved a higher TRL (5-7). For those, more demonstration activities at higher TRL (6-8) need to be achieved by 2030.

4.1.2 Materials and formulations design: integration with process design

Context: Currently, there is a disconnected design of materials from systems/processes design, rather than integrating materials properties as variables in a single, parallel design process. Incorporating process design and model-based materials is envisioned as a design paradigm change. Processability, physicochemical characteristics, safety, sustainability and recycling/re-use can then be considered as factors from the design phase. The different stages of materials and products development will therefore become seamlessly connected (process-structure-property relationships becoming established).

Specific challenges:

- Large margin of error for performance prediction with current methods (e.g. atom-scale computational catalysis optimisation);
- Enhance the capability of performance-based simulations over extensive materials physical testing and in parallel improve on multi-scale measurements and characterisation tools and methods. Empirical design curves are static and unable to easily and readily adapt to changes in the final product or modifications in process requirements. Multi-scale dynamic models to be used to support empirical models by providing molecular descriptors that contain more scientific information compared to just recipes and process conditions;
- Enhance existing types of models and methodologies (e.g. data-driven, deterministic, probabilistic) to become more robust, interoperable and adaptive. Empirical models must be improved by supervised machine learning from interpreted (labelled) data;
- Tackle technical complexity by bridging conventionally siloed experts and design stages throughout the RD&I pipeline. Build interdisciplinary research frameworks, leveraging skills in materials science, integrated engineering design, data analytics and computational methods;
- Modelling processes are often not universal (e.g. predictive design in 3D printing);
- Development/improvement of models for complex processes (e.g. biorefining, industrial symbiosis, and complex product formulations).

Specific expected impact: Combining process and materials modelling will achieve a significant impact on reducing the time and cost required for process development.

IMPACT EXAMPLES:

Example 1: The integration of materials modelling methodologies and knowledge-based systems with business process for decision making. The proposed concept moved towards a new paradigm of material and process design by developing and implementing an integrated multi-disciplinary, multi-model and multi-field approach together with its software tool implementation for an accurate, reliable, efficient and cost-effective prediction, design, fabrication, Life Cycle Engineering (LCE), cost analysis and decision making.[252]

TRL(now) & TRL(2030): Materials and formulations design/modelling integrated with systems/process design are currently at a low TRL (1-3). More research on exploring integrated material and process modelling as well as new methods for developing better algorithms need to be considered by 2030.

4.1.3 Design of reactors

Context: Reactor design, especially complex reactor systems (e.g. continuous flow, 3D-printed reactors, electrochemical, membrane and modular reactors – see **Chapter 3**), highly benefit from digital technologies by improving the design and thus increasing the quality of the scale-up output. By using digital technologies, `digital twins' of reactors can be designed and studied, reducing the high CAPEX and OPEX scalability risks involved.

Specific challenges: Similar to process and materials' modelling challenges (**sections 4.1.1 and 4.1.2**), integrating data-driven model approaches and the improvement of empirical models, are also highly relevant to the rational design of complex reactor systems.

4.1.4 High-throughput screening (HTE) methodologies

Context: Massive parallel testing/experiments can determine optimal process/materials combinations to accelerate R&D. This allows for an increased experimental load without subsequently increasing personnel costs or development time. This shortens the time to market for new products, improves product and process optimisation, and thus impacts the quality output of R&D laboratories.

Specific challenge(s):

- Even if high-throughput methodologies are currently in use for materials optimisation, its widespread adoption is challenging, thus a reduction in CAPEX is targeted;
- Fast sensing technologies may be improved to be able to detect a large variety of molecular structures, ranging from small molecules to complex polymers. Methodologies that link physical and molecular parameters are needed. New HTE methodologies should also aim at incorporating multi-modal sensors assessing "physical parameters";
- Adoption of high-throughput experimentation and machine learning for materials discovery and/or process optimisation are needed.

4.1.5 Robots for laboratory experimentation

Context: Beyond large-scale production, robotics is transforming how researchers gather and understand data, perform experiments and create new technologies. Robots automate research tasks and work, thus accelerating RD&I, increasing process transparency and robustness, whilst also contributing to human safety within labs.

Specific challenge(s): Better integration and continuous training of robots for various R&D tasks whilst improving human/robot interfaces. A large amount of different data sets is needed; and standardisation is currently missing.

4.1.6 R&D data management from multiple sources

Context: The ever-growing amount of RD&I lab data calls for improved data management to quickly harvest and improve the value generated from multiple data sources. These include searching and exploring very large chemical datasets through indexing and approximate processing, which contributes to accelerate R&D and increases process transparency and robustness.[253]

Specific challenges:

- Data systems processing of large, fragmented and variable data that can diverge by application and source;
- Inhomogeneous data quality and the large numbers of interconnected systems is the reality in which these data are used for automation and AI, the impact of bad quality data can have a larger negative effect from R& D to production and supply chains;
- RD&I data standardisation is missing. Chemical companies often lack the internal infrastructure, governance and processes to manage R&D data integrity throughout their lifecycle and address growing data vulnerability effectively;
- Imbed and enforce data integrity and security throughout R&D—while adapting existing investments in cybersecurity.

Specific expected impact: R&D data are used by chemical companies to speed up R&D efforts and control operations. Not surprisingly, 82 % of chemical industry respondents agree that as organisations rely on data-driven decisions, the issue of data integrity will grow exponentially.[254] Addressing the issue of data veracity from multiple and fragmented sources will enable the efficient use of AI-driven experimental design.

IMPACT EXAMPLES:

Example 1: Development of batteries for rapid charging using advanced approaches like density functional theory calculations in combination with machine learning and Artificial Intelligence to analyse big data collected from characterisation, synthesis and testing.[255]

TRL(now)&TRL(2030): Advanced R&D data management to address some of the above challenges has achieved a TRL 3-5. More demo activities at higher TRL (6-8) need to be achieved by 2030.

4.1.7 Virtual and augmented reality in laboratory environments

Context: Virtual and Augmented Reality can be achieved by using devices like smart glasses or interactive displays (e.g. smart surfaces).[256] These can bring highest impact by improving safety and efficiency of laboratory experiments.

Specific challenge(s): The registration problem remains a challenge as augmented reality implies using a complex suite of sensors that can track the user position and points of attention and a good understanding of the 3D-environment. A challenge is the difficulty to wear devices for several hours during lab experiments.

4.2 Process Analytical Technologies (PAT)

Context: The development and wide implementation of new sensors for batch and continuous processes is a key enabler to further progress on control, optimisation and automation of chemical processes. Such advanced PAT-technologies for real-time process monitoring, based on high-resolution analytical technologies, need to be suitable to be applied in complex reaction conditions (e.g. high-viscous, multiphasic, corrosive, scaling) and at the same time be reliable and accurate, robust, fast, contactless, intelligent, self-optimising, connected and affordable. Such new measurement systems, fully integrated in the automation environment of chemical plants, must be able to measure all relevant physical process variables but also perform analysis on the physicochemical properties of reactants, intermediates (e.g. particle size, structure of molecules-including isomers) and final products to feed reliable data into the model-based control and optimisation systems. A broad set of PAT technologies have already found their way into standard operating units within the chemical Industry. PAT can be applied in a wide range of applications, including continuous flow-reactors, batch-reactors, modular processes, water treatment, biotechnological processes, upstream/downstream processes to cope with feedstock-mix (e.g. waste/biomass), process monitoring for material deposition (e.g., for coatings or 3D-printing processes), extending to the digital retrofit of brownfield plants and sites.

Market, overall expected impact: PAT contributes to reduced production costs, greater efficiency, more reproducible results, and faster scale-up, whilst enhancing workforce capabilities and further improving health and safety.

Process analytical technologies (PAT) address several **Horizon Europe (HEU) clusters and areas of intervention areas:** 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Next generation internet' 4.6, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and industrial facilities with space in energy transition' (5.4), 'Seas, Oceans and inland waters' (6.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7) and 'Cybersecurity' (3.3), mainly by the following factors:

- **Improved production efficiency** by integrating PAT, which allows to better understand chemical processes and feed data into process models. This can help to quickly process data and predict and control product quality during the process, improving on OPEX;
- **Facilitate the use of alternative carbon feedstock** by accurately measuring feedstock composition/quality as the input of a process;
- **Improve safety of processes** by automating the analysis of different parameters in a continuous mode, and the early identification of any risks regarding the stability of a process (e.g. pressure, temperature, by-products);
- **Improved the environmental profile of a process** by integrating PAT, which allows to reduce waste and resource-consumption, achieving 'green' processing.

Horizontal challenges:

- Broader uptake of PAT-technologies for further optimised processes (e.g. developing processes with measurement and control capabilities that compensate for process variability);
- Increase trust in the quality of measurements and improve on the acceptance of new technologies by plant managers and operators;
- Increased resolution for monitoring in highly-advanced analytical separation technologies;
- Advanced PAT needs to be made more affordable (CAPEX reduction);
- Sensors which are energy efficient during operations;
- Incorporation of increasingly large volumes of data efficiently into PAT-systems with new generations of techniques for data cleaning and verification;
- Develop technologies which are more sensitive, robust and having the ability to detect properties and molecular compositions over a wider range of parameters;
- Sensors which deliver high-quality data, which can detect changes on-line and in real-time while being in a (low-) cost range;
- Low sensor maintenance requirements (e.g. plug-and-operate, incl. self-calibration);
- High sensor reliability (e.g. in demanding industrial environments: high temperature, high-pressure, explosive atmospheres, fouling, scaling, corrosive environments, abrasion, hazardous chemistry) for a long service life;
- Integrated sensor platform, able to measure more than one property in-situ and simultaneously;

- Integrated technologies in-situ, creating a fundamental understanding of chemical processes by obtaining online information (e.g. catalyst surface monitoring, or reaction products composition);
- Miniaturised, robust, potentially even handheld, easy to produce technologies with digital read-out;
- Improved technologies in support of novel processes, e.g., (3D-) extrusion/printing moulding or coating.

SUSCHEM PILLARS – MULTI-KETS:

PAT is expected to have a strong horizontal impact on RD&I in **Advanced Materials (Chapter 2)** and especially '3D-printable materials (2.2)' and **Advanced Process Technologies (Chapter 3),** highlighting 'Modular production (3.2)', 'Industrial biotechnology 3.10', 'Waste valorisation process technologies 3.11' and 'Process technologies for advanced water management 3.12'.

Within **Enabling Digital Technologies**, the relevant topics include: 'Laboratory 4.0/ Digital R&D (4.1)', 'Cognitive plants 4.3', 'Advanced data analytics and Artificial intelligence 4.4' and Predictive maintenance 4.5'.

RD&I Actions

4.2.1 PAT for continuous flow reactors and modular processes

Context: Analytical instruments used for PAT measurements are typically advanced analytical instruments to characterise a process sample. Examples of these include: (Fourier-transform) near- or mid- infrared spectroscopy (FTIR), Terahertz (THz) spectroscopy, Raman spectroscopy, mass spectrometry, and focused-beam reflectance measurement. More advanced technologies include the development of process sensor technologies for a wide range of applications. For instance, in the continuous manufacturing of platform chemicals, e.g. bio-based, real-time monitoring of the physical properties and molecular composition is crucial to secure product quality and process control. Novel, reliable and cost-efficient PAT for continuous processes, combined with simulation capabilities, will generate the basis to improve process control and thus plant operation reliability. Cyber-physical systems, applied in complex plants, will address the recognition of unusual situations in a continuous production manner, the proposal of adequate measures as well as the monitoring and integrating environmental targets (e.g. resource efficiency, energy consumption, emissions) but also high-level supervisory control to support process operators and engineers towards process intensification. With the large variation of feedstock composition, in some cases dramatically influencing the final product quality, continuous online upstream monitoring is crucial. The increased complexity of "downstream" continuous flow processes, on plant or even chemical site level, puts an enormous pressure on the performance of the PAT measurements, with several challenges: universal detection, low concentrations of pollutants and above all the diversity of the chemicals as process output. Furthermore, PAT can contribute to modular production and smarter water treatment systems by implementing real-time online sensors lower cost and ease of operation sensors or 'plug-and-operate' sensors.

Specific challenges:

- 'Separation power" for the continuous monitoring and measuring of multiple compounds, including variable feedstock components (biomass, waste), chemical reaction intermediates and products/ by-products;
- Online PAT-technologies able to detect a large variety of biomolecules, e.g. peptides, sugars and vitamins, as well as pH, oxygen content and other classical parameters;
- Online PAT-technologies able to detect a large variety of chemicals, like metals (catalyst) in various oxidation states, and small molecules;
- Sensors for parameters affecting (online-) water processes control (e.g. corrosion, scaling and/or fouling) and quality control (e.g. micro-pollutants, microorganisms, toxins and algae);
- Creation of sensor networks to control water systems and to collect operation relevant data for a dynamic operation of (waste-)water treatment systems;
- In-line sensors for continuous processes to provide maintenance-relevant data for predictive maintenance;
- Miniaturisation of sensors at affordable cost for modular production.

Specific expected impact: PAT technologies are key to achieve the conversion from batch to continuous processes, with a large spectrum of advantages on CAPEX, OPEX, safety and process flexibility, extending to modular production, with applicability on the synthesis of chemicals, being small molecules, biomolecules or polymers. PAT technologies in high throughput experimentation platforms are the basis of the design of new processes.

IMPACT EXAMPLES:

Example 1: €265 million/year financial savings, more than 490,000 t/year CO_2 emissions reduction, and 176,000 t/year less consumption of non-renewable raw materials in the related industries (complex organic synthesis, specialty polymers, and formulation of complex liquids) in Europe by introducing PAT (e.g. new online sensors with novel capabilities, novel closed-loop control methods for flexible operation and high-quality levels) that allow the continuous production of high-value products in flexible, intensified continuous production plants.[257]

Example 2: Development of PAT based on spectroscopy and Micro-Electromechanical Systems (MEMS) for inline rheology measurements, coupled with process modelling, leading to a closed-loop and tight real-time process control and optimisation, achieving more than 10 technology demos.[258]

TRL(now) & TRL(2030): The development of conventional PAT-technologies has achieved a relatively high TRL (5-8), especially for batch processes. The integration of PAT into continuous flow and modular processes as well as connecting PAT with closed-loop process control systems is at a relatively low TRL (2-4), requiring significant RD&I efforts by 2030.

4.2.2 Inline process monitoring for material deposition (3D-printing processes)

Context: Additive manufacturing (AM) technologies have gained significant importance from prototyping applications to the direct production of end-use parts with functional property and quality requirements. While different technologies such as Fused Filament Fabrication (FFF) and Powder Bed Fusion (PBF) focused more on the production of a specific shape rather than acquiring targeted intrinsic properties (e.g. multi-material printing). In addition, such production still lacks repeatability, reliability and proven quality control (QC) procedures, especially for inline monitoring.

The failure of AM parts is still often steered by more or less random printing errors. Post-printing quality control measures are extremely cost intensive. So far, typical polymer AM processes only monitor machine operation parameters such as temperature, gas flow rates or position of machine axes. There is only very limited close-loop control of relevant processing parameters as a function of the resulting properties of the printed part. As parts are produced layer-wise, a proper process control of actual conditions during material addition and activation needs to be put in place through PAT technologies.

Specific challenges:

- Integrate tools for the active control of the full manufacturing process, beyond visual control, with real-time information to act preventively before possible deviations occur;
- Inline process monitoring for functional bio-based 3D-printed polymers, dual/multi-material 3D-printing, and one-step polymerisation and 3D-printing processes;
- Incorporation of PAT technologies as standard or optional equipment especially in machines with more industrial characteristics.

4.3 Cognitive Plants: (Real-time) Process Simulation, Monitoring, Control and Optimisation

Context: Increasingly, process understanding is linked to operational excellence, preceding the full control of production processes. The switch from large-scale batch production to more sustainable and flexible continuous production increases the need to develop integrated physical- and soft-sensors measurements combined with advanced modelling of all critical process/product quality attributes. Automated feedback and closed-loop control of the process/product parameters ensures efficient control and stability of processes, reducing product variability, thereby preventing products being rejected further down the supply chain on adjacent processes. Operations need to understand process problems in a quick way to achieve operational excellence in complex processes.

Linking big data to real-time process simulation will enable more agile processes, better integration of supply chains, greater transparency on environmental issues, and optimal real time decisions for energy efficiency, in a wide range of processes, including chemical- biotechnological-, biorefining-, recycling-, modular-, intensified-processes, and water treatment as well as other process systems extending to the retrofit of brownfield sites.

Market, overall expected impact: Optimisation of a few important parameters in real-time could reduce energy costs by 4 to 5 % and increase process efficiency by 90 %.[259]Cognitive plants with closed-loop control will be crucial to allow for integration of upstream and downstream parts of the value chain, monitoring and real-time decision-making, accounting for environmental impact and energy efficiency; whilst enhancing workforce capabilities and further improving health and safety.

Cognitive plants: (Real-time) process simulation, monitoring, control and optimisation address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Next generation internet' 4.6, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and Industrial facilities in energy transition' (5.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7), 'Protection and security' (3.2) and 'Cybersecurity' (3.3), mainly by the following factors:

- **Improved process efficiency by integrating real-time process simulation, model predictive control and digital twins** that go from full-scale **processes** to plant **simulations** (both design and operation phases);
- **Improved safety and environmental performance profile of chemical processes** through integration of LCA parameters in process models as a key enabler for real-time monitoring and optimisation of resource and energy efficiency. This will result into achieving much greater agility of processes to respond to variations in feedstock and energy, factors of rising importance in energy transition and circular economy operation models;
- **Use of big data for AI-driven and hybrid models applicable to process/plant simulation and control** will create challenges and opportunities for computing, next generation connectivity, data management and cybersecurity capabilities within the industry.

Horizontal challenges:

- Improving management of big data to support operational decisions with systematic incorporation of uncertainty in feedstock composition and equipment parameters, handling discrete decisions for large scale problems. This requires faster computational power to enable real-time decision making based on very large-scale integrated models with complex physico-chemical predictive capabilities to ensure good quality predictions;
- More RD&I on building chemical process-related models along with AI and improved user-oriented capabilities;
- The production of more complex materials and molecules requires greater predictive capability in the fundamental models and their parameters using better understanding from recent developments in fundamental science. This will require more efficient and robust solution algorithms to ensure optimal solutions can be obtained in reasonable time scales.

SUSCHEM PILLARS – MULTI-KETS:

Advances in 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation' is expected to have a strong horizontal impact on RD&I in **Advanced Process Technologies (Chapter 3)**.

Expected advances in AI, big data, IoT, will enable more advanced real-time process simulation, monitoring, control and optimisation, and therefore its implementation by the chemical and biotech sectors. Within **Enabling Digital Technologies**, the relevant topics include: 'Coordination and management of connected processes at different levels 4.8', 'Process Analytical technologies (PAT) 4.2', 'Advanced data analytics and Artificial intelligence 4.4', 'Digital support of operators and human-process interfaces 4.6', 'Predictive maintenance 4.5' and 'Data sharing platforms, data security 4.7'.

RD&I Actions

4.3.1 Process Modelling/Process Simulation/Model Predictive Control

Context: Process modelling using fundamental principles provides the basis for simulation, optimisation and control of chemical processes and has enabled huge gains in development time, operational productivity, and managing risk and uncertainty. A new generation of tools is needed to systematically produce models of greater accuracy, enabling the seamless incorporation of the increasingly vast amounts of available data to embrace models of different type, language and fidelity.

Specific challenges:

- Develop models to enable 'auto-adaptive' processes in real-time – use of verified (big) data streams from current and historic process operations;
- Developing and integrating AI-based models which can be 'easily' updated under operational conditions with reduced needs for detailed analytical (rigorous) models;
- Ensure that data are highly reliable, therefore data generation (e.g. by sensors), data robustness, data quality, and data access need to be improved widely;
- Overcoming the modelling bottleneck by improving model re-use across different processes, developing strategies for more efficient model maintenance and (self) adaptation;
- Combining use of rigorous models and data analytics for the recognition of unusual situations in complex plants and the proposal of adequate measures or next steps;
- Further develop dynamic simulations; large-scale non-linear, dynamic numerical optimisation models, discrete-event simulations, models with discontinuities, surrogate models, integrated process models, hybrid modelling, physics simulations, and steady-state simulations, etc.;
- Develop models and solutions for flexible and adaptive use of different types of energy (renewable energy grids) and define suitable optimisation strategies which could help to find optimal solutions, coping with renewable energy intermittency;
- Developing integrated models for new processes based on constraints linked with circular economy and feedstock composition fluctuations, exploring the full benefits and challenges;
- Acknowledging the role of the humans in the operation of plants (e.g. how can their knowledge and experience be optimally combined with advanced process control algorithms and optimisation; how can humans supervise complex computer-based solutions);
- At-a-glance visualisation of the health of units and equipment coupled with modelling/machine learning for anomaly detection as a basis for all dynamic simulation modelling to enable operators/plant engineers to assess problems quicker and stay ahead of potential issues in the plant;
- Digital twins for plants, processes and products which can communicate to each other in a highly flexible way e.g. to solve complex production problems in a self-organised manner;
- Generate accurate, curated and readily accessible operational data to support both routine (automated, autonomous) workflows and analytics-supported optimisation.

Specific expected impact: Process Modelling/Process Simulation/Model Predictive Control to achieve a greater reliability of processes by making them safer and more predictable, thus enabling better management of risk and uncertainty. This can in turn, optimise the whole supply chain through integrated models that will result in optimal economic and environmental performance for customers.

IMPACT EXAMPLES:

Example 1: Integration of machine learning functions to improve process simulation and optimisation of critical process industries (power companies, refineries, ceramic industry, pulp and paper, chemical), showcasing a 10 % reduction of energy and improved resource efficiency for several important applications: for example, in biogas production from waste water treatment plants. The impact extends to doubling of production output and reduction of electricity demand by 50 %.[260]

Example 2: The combination of advanced process models and optimisation techniques resulted in an improvement in process

economics of tens of millions of Euros over the original design, which was performed using traditional process simulation techniques.[261]

TRL(now) & TRL(2030): Technologies for process modelling/process simulation/model predictive control are currently at TRL (2-6). Specific focus is recommended on combining physical principal models with advanced AI-based algorithms to prove large scale process adaptability and robustness. More demonstration activities at higher TRL (6-8) need to be achieved by 2030.

4.3.2 Environmental performance optimisation: Resource and energy efficient plants

Context: Real-time monitoring and optimisation methods should allow operators to monitor resource efficiency, with environmental implications, during daily operations of large production plants to influence the operational decisions such that the plant efficiency is optimised, and the environmental footprint is constantly minimised. Key environmental factors are energy consumption, water consumption, CO_2-emissions, pollutants, and waste generation, amongst others. Towards reaching this goal, indicators must be defined to provide meaningful information about the resource efficiency over different timescales and connect these indicators with new analytical measurements, extending to process parts that may not have been previously included in the process model/simulation. Based on the new indicators, decision support and guidelines for the operating staff must be developed. The indicators will provide a multi-dimensional field in which the operators are enabled to decide on the optimal status of the production process.

Specific challenges:

- Integrating more LCA parameters in monitoring;
- Monitoring of environmental targets like energy and/or water consumption, CO_2-emissions, pollutants, waste etc. into the plant control systems;
- Enable 'self-driven' and 'self-organising' production with optimal resource and energy efficiency;
- Apply monitoring and modelling to ensure energy efficiency and meeting other environmental targets at different levels: from plant, site, industrial parks, municipalities to across industries (industrial symbiosis);
- Develop methods for decision support for operating staff towards higher resource efficiency.

Specific expected impact: For 2030, all processes should have the ability to be monitored in real-time to allow for environmental plant performance improvements. The development of more sophisticated process models for large scale real-time monitoring and optimisation and especially the integration of LCA-parameters into such models is necessary. This will enable the industry to realise further significant resource and energy efficiency improvements, greater transparency of operations, more sustainable operations and process improvements in faster and safer ways.

IMPACT EXAMPLES:

Example 1: Development of low-cost MEMS-NIR spectroscopic and granulometric analysers, smart sensors for batch and continuous processes, and integration of these into a global control platform with the chemometric tools and the predictive software. This delivered an integrated process control platform to enable near real time closed-loop process control to operate industrial processes at their optimum, both economically and environmentally.[262]

Example 2: Economic gain of between € 1-5 million per annum equivalent to 3-5 % of cost savings and a reduction of greenhouse gas emissions of 3.5 % by identifying resource efficiency indicators that can support operational decisions in processing plants using real-time data and the implementation of dedicated online decision support systems.[263]

TRL(now) & TRL(2030): Technologies for (real-time) monitoring and optimisation for resource efficiency and plant performance improvements are currently at TRL (2-6). Specifically, the integration of LCA-parameters into process models is still on relatively low TRL-levels and lacking plant implementation. More RD&I on demonstration activities at TRL 5-7 to apply these technologies in both new and existing production units needs to be considered by 2030.

4.3.3 Digital Twins/Digital Process Development/Plant Engineering

Context: Digital Twins will enable a digital transformation in the way chemical industries operate. Having a digital twin of the full process and plants enables engineers to simulate implications of changes in process parameters in a more holistic way. Process modelling together with data science is required for such digital twin development. Once a digital twin is developed all the

techniques of control and optimisation together with data cleaning and statistical analysis can be deployed to obtain optimal performance conditions. The future should enable three-dimensional real-time visualisation using virtual reality, where appropriate.

Specific challenges:

- Further research on simulation of production processes, processes for formulated products and whole smart plants;
- Enhancing capabilities to significantly lower the effort and cost of generating digital twins of plants considering existing and new plants through the interoperability of models and tools, the standardisation of taxonomies and the extended adoption of semantics techniques;
- Developing digital twins for digital engineering and plant operation management in an integrated way along the whole life cycle of a plant, covering product and process development, plant engineering, procurement, plant construction, commissioning, later operation, as well as plant flexibility, extensions and reuse for next generation and new products;
- Handling process simulation, data visualisation and asset management together in one digital twin;
- Managing large volumes of unstructured data with advanced statistical techniques feeding into digital twins;
- Integrating 'Virtual Reality' tools in a computationally efficient ways to enable real-time visualisation and large-scale scenario planning into digital twins;
- Use digital twins for plant control training of operation staff.

Specific expected impact: Digital Twin/Digital Process Development/Plant Engineering will allow the efficient simulation of process parameters accelerating the design and the efficiency of the utilisation of plant assets. Furthermore, digital twins contribute to better safety of operations through prediction and early identification of possible root causes of major process disruptions. Going beyond process and plant operation improvements, offline and online supervised training of operation staff contributes to the efficiency and safety of the plant control and operations.

IMPACT EXAMPLES:

Example 1: Use of mathematical models and Machine Learning approaches to develop data-based models for different processes. These models have the potential to become part of future digital twin implementations in two use cases (steel and copper industries).[264]

Example 2: Digital Twin applications in the petrochemical industry to improve operation, maintenance and safety, for example in chemical plants and offshore platforms.[265]

TRL(now) & TRL(2030): The development of Digital Twins integrating a number of different models to simulate a whole production process or a plant is currently at lower TRLs (3-4) and a key challenge moving towards 2030. Additionally, both process and plant engineering development need to be implemented through connected digital models to achieve demo-scale developments.

4.4 Advanced (big-) Data Analytics and Artificial Intelligence

Context: (Big) data technologies including Artificial Intelligence (AI and Machine Learning (ML) algorithms have the potential to assist the chemical sector to achieve disruptive transformations both in performance and value generation[266,267] Data-driven innovation in the chemical industry of the future combines data inputs (historical and real-time) from connected sensors, data from research, process development, data from analysing products and product applications, data from raw materials, data from marketing/sales/customers and other operational and business relevant information. To effectively train AI-algorithms, large amounts of reliable data from different often siloed sources are required, therefore data access and generation (e.g. by PAT), data robustness and data quality need to be improved widely. Decision making, automation and control based on AI-algorithms will have a massive impact in multiple areas of the chemical industry: research & development, production, supply chain, sales and logistics. The integration of predictive and prescriptive data analytics, data processing architectures, interactive visual analytics and data management into advanced processes, result into advanced process control and efficiency of operation. Moreover, advanced data analytics will bring an additional dimension of implementing knowledge and information on market trends to finetune production according to predicted customer needs.

Market, overall expected impact: According to a recent study[268], technologies to utilise Big Data will deliver great value to enterprises by decreasing expenses (49.2 %) and creating new trends for innovation and disruption (44.3 %) with an estimated CAGR of 13.2 % during 2018-2022. Optimisation using data, extensively applied in all stages of the value chain, provides the objective base for value extraction. The physical plant becoming linked to its digital twin as data becomes a driver for more reliable and precise models at the base of predictive and autonomous processing.

Advanced data analytics and AI application in the chemical sector will address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Energy grids' 5.3, 'Buildings and Industrial facilities in energy transition' (5.4), 'Seas, Oceans and inland waters' (6.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7), 'Protection and security' (3.2), 'Cybersecurity' (3.3), and 'Environmental and social health determinants' (1.2) mainly via:

- **Implementation of AI-based advanced data analytics in the chemical sector**, from infrastructure to interactive visualisation, to provide efficient mechanisms to optimise research, operational and business processes by supporting decision-making capabilities (economic, safety, environmental and technical factors) by correlating information from multiple sources. These advantages become increasingly relevant for complex and novel processes such as those for waste valorisation to chemicals, biorefining and the integration of the energy sector, amongst others.

Horizontal challenges:

- **Data-processing architectures and data veracity establishing for high volume/dynamic (big-) data** generated by the chemical industry;
- **Transform 'Big, Fast and Unstructured Data' from multiple sources into decision-making information** through reliable data-driven models;
- **Apply sensor data analytics and advanced visualisation for real-time and historical industrial data**, prescriptive analytics, and advanced decisions support thus enabling operators/humans with capabilities for 'multi-dimensional' thinking and decision making;
- **Using cloud-based networks to communicate** on sensor-, plant-, site-, remote-site levels and enable user-friendly AI-computing access possibilities which are providing abilities for on-demand provision of extraordinary scalable high-performance computer resources with manageable technical hurdles and financial efforts;
- **Convergence of data analytics and business intelligence**, addressing the gap in industry between process-generated data and business-data relevant to feed into AI-analytics.

SUSCHEM PILLARS – MULTI-KETS:

'Advanced (big-) data analytics and artificial intelligence' is expected to have a strong horizontal impact on RD&I in **Advanced Process Technologies (Chapter 3)**.

Within **Enabling Digital Technologies**, the relevant topics include: 'Laboratory 4.0-Digital R&D (4.1)', 'Cognitive plants, (real-time) process monitoring, control and optimisation 4.3', 'Coordination and management of connected processes at different levels 4.8', 'Process Analytical technologies (PAT) 4.2', 'Digital support of operators and human-process interfaces 4.6', 'Predictive maintenance 4.5' and 'Data sharing platforms, data security 4.7'.

RD&I Actions

4.4.1 AI and Machine Learning

Context: Implementation of machine learning (ML) algorithms for better and faster decision making, predictive maintenance, and consistent improvements in process control and process safety.

Specific challenges:

- Combine advanced machine learning techniques with fundamental models, based on physical principles; currently data analytics are used decoupled from fundamental knowledge, thus producing less sophisticated insights;
- Data processing architectures for high volume and dynamic data;
- Reduce data pre-processing efforts before data AI algorithms can be effectively implemented. Currently, this is the bottleneck for any application e.g. production data requires a lot of (often manual) pre-processing by experts;
- Develop tools and methods based on models, sensors, diagnosis and data analysis allowing remote control of equipment, prediction and prevention of failures, identification of trends and avoidance of any loss of efficiency and unwanted stoppages;
- Extend ML for anomaly detection to reduce unplanned outages, equipment (valves, pumps, heat exchangers, motors, etc.), maintenance scheduling, mobile platforms for maintenance/remote control, asset management systems, smart meters in production.

Specific expected impact: All chemical processes should increase the ability to be controlled and improved in real-time, utilising pattern recognition to better predict plant and asset performance.

IMPACT EXAMPLES:

Example 1: Development of ready-to-use scalable online machine learning algorithms and interactive visualisation techniques for real-time predictive analytics to deal with extremely large data sets and data streams, taking the example of steel as a case study.[269]

Example 2: Development of a dynamic, distributed, self-adaptive and proactively configurable architecture for processing Big Data streams. It includes cloud-based self-adaptive real-time Big Data processing, and mobile stream processing, combining real-time Big Data, mobile processing and cloud computing research.[270]

Example 3: Predictive cognitive maintenance decision-support system to improve preventive maintenance and increase machines' in-service efficiency. It applies AI on real-time sensor data to track machine-tool performance and health condition.[271]

Example 4: Predictive and prescriptive maintenance framework systems for zero unexpected breakdowns and increased factories operating life.[272]

TRL(now) & TRL(2030): Currently, predictive and prescriptive analysis, using machine learning, is not widely used in the chemical industry, a paradigm shift should thereby take place by 2030, combining process innovation with the deployment of digital tools and data analytics.

4.4.2 Water data management

Context: Clean drinking water is scarce around the world. Therefore, further improvements in water usage and purification will have a global impact. Water data security and trust in sharing data, open format standards, merging data from private and public sectors and sharing data across industries will drive improvements in water usage and support addressing water scarcity issues.

Specific challenges:

- Flexible algorithms for data analysis to support water operation decision making, risk management, model development and use considerations on an integrated system level;
- Valorise big data and and Internet of Things (IoT) information (e.g. control systems for water networks), advanced technologies and capabilities (e.g. HPC – high performance computing) for quasi-real time data analysis, forecasting, visualisation and communication for advanced decision support and management;
- Development of digital process twins for industrial water management, connected with process control and manufacturing execution systems;
- Water data security, open format standards and trust in sharing data to share data across industries and to merge data from private and public sectors.

Specific expected impact: Appropriate water data management will have a global impact with a strong benefit for societies, accounting for water scarcity, but also across different industrial sectors. For example, the agri-food sector will benefit from efficient water usage, process industries will be able to perform efficient water usage and minimise waste, boosting productivity and environmental performance.

IMPACT EXAMPLES:

Example 1: Holistic approach for water management in the process industry using innovative technology solutions from EU companies to increase water and resource efficiency in the industry.[273]

Example 2: Localisation, visualisation and analysis of urban water data coming from sensor technologies to monitor in real-time water resources and provide decision support for water management.[274]

TRL(now) & TRL(2030): Current water data management technologies are at TRL 3-4 since commercial solutions do not consider all the available data sources. As more data is gathered, the algorithms and commercial tools to efficiently manage water data are expected to reach demonstration levels by 2030.

4.5 Predictive Maintenance

Context: Predictive maintenance (PdM) refers to monitoring the performance and condition of equipment during normal operation to reduce the likelihood of failures.[275] Historically, predictive maintenance was done with equipment manufacturer recommendations, condition asset monitoring, and human know-how. However, predictive maintenance costs could account for up to 70 % of the plant's overall production costs.[276] The concept of predictive analytics will greatly improve the overall shutdown planning and maintenance of a unit. Predictive analytics uses AI by building a model of "good data" and running continuously comparing the current snapshot of data patterns with the historically good patterns. Once the patterns start to deviate from normal then a subject matter expert can inspect the equipment. Predictive analytics and advanced machine learning can also be used to predict unit process performance by utilising the same general methodology at a much larger scale. Hence, incorporating digital tools (e.g. big data analytics, Industrial IoT sensors, AI) into predictive maintenance is realising tremendous results and value for companies.[277] These techniques encompass predictive maintenance of equipment, production systems and asset management systems.

Market, overall expected impact: Through predictive maintenance, integrated with digital tools, chemical companies can increase production yields, with the effect of better energy and resource efficiency and reduced production costs. It increases overall plant availability by minimising unplanned stops of production. A great advantage of applying predictive maintenance is to optimise the scheduling of connected processes.

Predictive maintenance addresses several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' (4.4), 'AI and robotics' 4.5, 'Next generation internet' 4.6, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and Industrial facilities in energy transition' (5.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7), mainly by the following factors:

- **Reduced costs and improved efficiency** by integrating digital tools in predictive maintenance, to predict equipment failures for equipment, production systems and asset management systems;
- **Improved maintenance accuracy** through digital tools in predictive maintenance.

Horizontal challenges:

- Further and broader uptake and implementation of predictive maintenance concepts (hardware and software) into the chemical production environment, currently especially challenging for retrofitting existing assets (CAPEX constraints);
- Develop optimal maintenance strategies in combination with improved scheduling to enable self-driven and self-organising production;
- Integration of data on the condition of the equipment into the overarching process control and optimisation systems.

SUSCHEM PILLARS – MULTI-KETS:

Predictive maintenance (PdM) is expected to have a strong horizontal impact on RD&I in **Advanced Process Technologies (Chapter 3)**, especially for 'Tolerant and intensified reactors and processes feedstock variability / energy fluctuation / electricity fluctuation (3.1.1, 3.1.2, 3.1.3)'.

Within **Enabling Digital Technologies**, the relevant topics include: 'Cognitive plants (real-time) process monitoring, control and optimisation 4.3', 'Advanced data analytics and Artificial intelligence 4.4', 'Process Analytical technologies (PAT) 4.2', 'Coordination and management of connected processes at different levels 4.8', 'Digital support of operators and human-process interfaces 4.6' and 'Data sharing platforms, data security 4.7'.

RD&I Actions

4.5.1 Predictive maintenance of equipment/production assets

Context: Predictive maintenance of equipment/production assets consist of developing tools and methods based on models, sensors, diagnostics and data analytics allowing remote control of equipment, prediction and prevention of failures, identification of trends and avoidance of any loss of efficiency and unwanted stoppages. Examples include the use of smart positioner information to know the health of valves; online monitoring of pumps; comparing real-time performance with manufacturers' pump curve and alert on deviations; or the use of machine learning for leak detection of heat exchangers or for preventing

motor failure. These techniques can help with outage planning for maintenance, damage reduction, prevent unplanned shutdowns, or safety improvements.

Specific challenges:

- Developing tools and methods based on models, sensors, diagnosis and data analysis allowing (1) remote control of equipment, prediction and prevention of failures, identification of trends and avoidance of any loss of efficiency and unwanted stoppages; (2) anomaly detection to reduce unplanned outages, equipment (valves, pumps, heat exchangers, motors, etc.), and (3) maintenance scheduling, mobile platforms for maintenance / remote control, smart meters in production networks and systems;
- Developing predictive models is highly complex and requires the development of algorithms for prediction and prevention of failures and identification of trends;
- Predictive maintenance requires ongoing model 'maintenance' and monitoring, adjustments need to be continuously solved;
- Develop a predictive maintenance platform that prioritises looming equipment failures seen with machine-learning to properly plan equipment change-out or maintenance stoppages. This could include adding safety and criticality information into the automated decision making;
- Further deploy smart and connected sensors and equipment technologies to send information to an asset management system (AMS) or the cloud to alert maintenance and help with troubleshooting. As more assets become interconnected, and with the IoT becoming ubiquitous, safeguarding access to critical equipment and adopting cybersecurity protocols while protecting connected assets is a key challenge.

Specific expected impact: Predictive maintenance to achieve a significant impact on reducing costs and improving efficiency and safety of the functioning of equipment and chemical production processes. Furthermore, all processes should have the ability to be monitored in real-time utilising pattern recognition capability to better predict plant and asset performance.

IMPACT EXAMPLES:

Example 1: Development of a universal and fully automatic machine learning solution for predictive maintenance of industrial equipment in the manufacturing sector able to reduce maintenance costs by 15-35 % by prevention of machine failure, improve resource management with a 5-15 % reduction in utility costs and increase stock rotation by 5-10 %.[278]

Example 2: Development of a platform based on nanosensors that measure the structural integrity of all the single components within the industrial plant in real-time, enabling the simultaneous measurement of multiple parameters (e.g. pressure, temperature, humidity, open-close cycles, micro-cracks, leakages, etc.) with high accuracy and sensitivity, providing the most accurate real-time monitoring of the whole industrial equipment.[279]

Example 3: Overall savings of up to 20 % per year for OPEX through the development of a novel Predictive Maintenance method, demonstrated in a coated paper mill. This method consists of new tools to adapt dynamically the maintenance and operation strategies to the current condition of the critical components in production equipment, enabling to find systematically the best maintenance strategy to maximise the availability of equipment and minimise maintenance costs.[280]

TRL(now) & TRL(2030): Predictive maintenance integrated with digital tools has achieved a TRL 5-7 in sectors such as the automotive sector. Similar progress should follow within the chemical sector, considering the complexity of chemical processes in regards to processing steps and process conditions (pressure, temperature, corrosivity etc.) and the respective effects on plant equipment. More demonstration activities are recommended regarding transitioning the implementation of predictive maintenance in chemical plants by 2030.

4.6 Digital Support of Operators and Human-process Interfaces

Context: Modern process technologies have become more complex, requiring highly qualified personnel to handle complex information streams. At the same time the importance of predictive maintenance increases to reduce unscheduled downtimes, identify (critical) process states and assess wear and tear of equipment. Intuitive human-machine interfaces to efficiently support people at the workplace thus become increasingly important. Technologies like smart glasses, augmented reality, data analytics, combined with smart hand-held devices provide a hitherto unknown availability of information, visualisation and interaction possibilities. The potential of the combinations of these technologies still must be explored. There will be a paradigm shift from the conventional control room to the provision of smart information, visualisation and offsite interaction both for the operator and the maintenance crew on the site. By providing pre-processed information, tailored to the current situation, decision taking in complex situations and safety at work will be strongly enhanced. This will be complemented by knowledge management technologies to represent either written (documented) information and/or the knowledge of experienced operators.

Market, overall expected impact: In the environment of 'Machine-to-Machine' and 'Human-to-Machine' (M2M, H2M), the 'humans-in-the-loop' concept is always central for operation control and management in the operation of plants belonging to process industries. Digital support of operators encompasses the optimum use of their knowledge and experience and providing support combining situation awareness and information provided by advanced control algorithms and optimisation. Such an approach empowers operators' actions through the extended adoption of wearable systems, augmented reality technologies and virtual reality-based training, improving dramatically safety and effectiveness in operations at the same time.

'Digital support of operators and human-process interfaces' address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'AI and robotics' 4.5, 'Next generation internet' 4.6, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and Industrial facilities in energy transition' (5.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7) and 'Cybersecurity (3.3)'.

IMPACT EXAMPLES:

Example 1: Human workforce to be more efficient as well as more creative by using augmented reality (AR) and AI technologies for real time feedback on processes that can be displayed in their AR glasses.[281]

Horizontal challenges:

- 'Humans in the loop': define the role of humans in the operation of plants, how can their knowledge and experience be optimally combined with advanced control algorithms and optimisation, how can humans supervise complex computer-based solutions;
- Design more intuitive systems for operators (e.g. dynamic data dashboards);
- Virtual environment/virtual reality for training of full production processes. Digital twins and plant models for learning purposes;
- Augmented reality, e.g. smart glasses for plant-operator interaction for enhanced plant safety;
- Enhanced operator's knowledge through data analytics/AI and machine learning;
- Interactive visual analytics.

SUSCHEM PILLARS – MULTI-KETS:

'Digital support of operators and human-process interfaces' is expected to be impacted by other RD&I areas within **Enabling Digital Technologies**: 'Laboratory 4.0-Digital R&D (4.1)', 'Cognitive plants, (real-time) process monitoring, control and optimisation 4.3', 'Advanced (big-) data analytics and artificial intelligence 4.4', 'Coordination and management of connected processes at different levels 4.8', 'Predictive maintenance 4.5' and 'R&D and technology transfer - collaborative data platforms (4.7.2)'.

4.7 Data Sharing Platforms and Data Security

Context: Data sharing often represents one of many steps in the digital transformation of a company or an institution. However, the lack of operating platforms for secure and controlled sharing of "closed" datasets (proprietary/commercial/industrial data) seriously limits the capacity of Europe to respond to the digitalisation challenge of the chemical sector. The relevance and efficacy of data sharing platforms in digitalising business capabilities for the chemical industry becomes applicable to enable connected value chains, industrial symbiosis, or technology transfer. Through 'Open Science', research communities are also moving towards a much more transparent environment for research results, with smart access to research data enabling innovation in industry, Academia and the full innovation ecosystem, including SMEs, start-ups and RTOs.

Market, overall expected impact: Building a European data economy is a key part of the European Commission's Digital Single Market strategy.[282] The EU intends to unlock the re-use potential of different types of data and its flow across borders to achieve a European Digital Single Market. Data sharing and reuse by multiple actors maximises value extraction and leads to the creation of new services and the emergence of novel business models. Data sharing platforms have great potential in improving collaborations across stakeholders with high expected results through assisting industrial symbiotic networks by enabling digital trust on sharing data related to transactions.

Data sharing platforms and data security technologies implementation in the chemical sector will address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Next generation internet' 4.6, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Energy grids' 5.3, 'Buildings and Industrial facilities in energy transition' (5.4), 'Agriculture, Forestry and the rural areas' (6.3), 'Seas, Oceans and inland waters' (6.4), 'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7), as well as 'Environment and social health determinants' (1.2) and 'Cybersecurity' (3.3), mainly via:

- **Improved collaboration and communication across value chains** by integrating raw material providers, manufacturers and customers, or even across different sectors (e.g. food, pharma, biorefining, waste management, energy) and other process industries (e.g. steel, cement) to enable industrial symbiosis via coordinated management of process operations, consequently, increasing resource and energy efficiency;
- **Improved information sharing between R&D networks** to enable efficient access to experimental data, fostering industrial deployment of results, but also promoting more collaborative and larger projects across companies, different players in the innovation ecosystem and even different sectors;
- **Increased the transparency** of how products are processed across value chains (from raw material origin to end use), will allow manufacturers to tailor production to customers in addition to enabling the management of resources as well as the transparent tracking of the circularity of their products.[283] This contributes to increasing resource and/or energy efficiency and thus reducing carbon and overall environmental footprint;
- **Improved decision making** by increasing data availability for sustainability assessment and safe-by-design for chemicals and materials;
- **Improved safety** of chemical products by building global repositories of publicly available information on chemicals.

Horizontal challenges:

- Establish a culture of 'digital trust' by the means of control on legal compliance;
- Implement cybersecurity to protect data assets;
- Ensuring safe methods for data, know-how and information sharing while retaining key elements of intellectual property to protect business positions.

SUSCHEM PILLARS – MULTI-KETS:

Data sharing platforms and data security technologies implementation in the chemical sector is expected to have an impact on RD&I in **Advanced Process Technologies (Chapter 3)**, especially on processes related to the integration of waste as feedstock: 'Waste valorisation process technologies 3.11' but also in 'Process technologies for advanced water management 3.12'.

Within **Enabling Digital Technologies**, the relevant topics include: 'Laboratory 4.0-Digital R&D (4.1)', 'Advanced data analytics and artificial intelligence 4.4', 'Predictive maintenance 4.5', 'Coordination and management of connected processes at different levels 4.8', and 'Distributed ledger technologies 4.9'.

RD&I Actions

4.7.1 Industrial data sharing platforms

Context: Industrial data sharing platforms support secured and controlled sharing of datasets: they contain machine-operation data, make them accessible to control applications, allow third parties to build services on that data, and automate data sharing with smart contracts. There is a strong need to build and integrate industrial data platforms to activate the data economy in important sectors such as the chemical industry, maximising data value extraction and leading to the emergence of new business models. As data sharing platforms are under permanent development, including for many applications for other industrial sectors, it must be ensured that platform implementation within the chemical sector is further strengthened, focusing on two main orientations:

- **Industrial data platforms enabling value chains integrated into the chemical industry** to allow data exchange between different stakeholders, resulting into more efficient business processes;
- **Industrial Symbiosis - waste streams databases/ platforms**: To unlock the full potential of industrial symbiosis, data value chains need to be built and data-driven waste/by-product valorisation and cross-sectorial resource/material reuse needs to be facilitated. (For further information, see 'Coordination and management of connected processes at different levels 4.8').

Specific challenges: See 'Horizontal challenges 4.7'.

Specific expected impact: Market, overall expected impact 4.7.

IMPACT EXAMPLES:

Example 1: Creation of an innovative Industrial Symbiosis (IS) platform, bringing together five key relevant sectors within the process industries: steel, cement, chemicals, minerals and engineering, enabling cross-sectorial collaborations and providing a wide range of technological and organisational options for making business and operations more efficient, more cost-effective, more competitive and more sustainable across process sectors. Mapping of potential industrial symbiosis streams (energy/ materials) and activities 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.[284]

Example 2: Creation of a centralised database for critical raw materials, offering to the recycling industry, producers, and policy makers information on mineral resources from extraction to end of life products with the ability to reference all spatial and non-spatial data.[285]

TRL(now) & TRL(2030): Technologies for enabling industrial data platforms have achieved a TRL 5. More demonstration activities at TRL 8 are recommended to prove the scalability and computational efficiency of methods for securing desired levels of privacy of personal data and/or confidentiality of commercial data by 2030.

4.7.2 R&D and technology transfer - collaborative data platforms

Context: Data platforms to share and exchange scientific knowledge, experimental data, know-how, tools and good practice provide effective communication among involved stakeholder researchers, resulting in shortening the timelines of an R&D pipeline, enhancing interdisciplinary research whilst also allowing for a much more transparent environment for research results. Smart access to research data will help innovation in and between industry, Academia and the full innovation ecosystem, including SMEs, start-ups and RTOs.

Specific challenges: See 'Horizontal challenges 4.7' and especially intellectual property agreements.

4.7.3 Cybersecurity

Context: In the era of data-exchange and value generated through data-ownership, the chemical industry must be considered as an important stakeholder in initiatives on industrial cybersecurity. The chemical industry should develop advanced security solutions to prevent misuses of stored data and attacks on plant control and wireless systems or cloud data in an environment where data are more and more geographically dispersed from the viewpoint of remote data-servers and manufacturing hubs.

Specific challenges:

- Develop mechanisms that measure the performance of ICT systems with regards to cybersecurity and privacy;
- Enhance control and trust of the consumer of digital products and services with innovative tools aiming to ensure the accountability of the security and privacy levels in the algorithms, in the software, and ultimately in the ICT systems, products and services across the supply chain;
- Original Equipment Manufacturers (OEM) to develop security-by-design applications instead of relying on separation for OT security.

Specific impact:
Achieve impact on tackling issues of threat detection, implementing countermeasures as well as real-time responses when needed. Thus, cybersecurity is taken up by the chemical industry to guarantee significantly increased cyber-security levels in daily operations for manufacturing facilities and other actors in the value chains.

IMPACT EXAMPLES:

Example 1: Development of a 'European Reference Network for Critical Infrastructure Protection (ERNCIP)' with the aim of providing a framework within which experimental facilities and laboratories will share knowledge and expertise to harmonise test protocols throughout Europe, leading to better protection of critical infrastructures and the creation of a single market for security solutions. This project consists of 12 working groups, some of them closely related to the chemical industry, e.g. Chemical and Biological Risks of Drinking Water, or Industrial Automated Control Systems and Smart Grids.[286]

Example 2: Development of modular solutions (technologies, tools and guidelines) and an integrated software platform for water systems protection to identify current and future risk landscapes and to co-develop an all-hazards risk management framework for the physical and cyber protection of water critical infrastructures. [287]

TRL(now) & TRL(2030): More demonstration activities are recommended to implement available cybersecurity solutions into the chemical sector, accounting for the complexity and high risk associated with its processes, large portfolio of products as well as the resulting cross value chain and cross-sectorial collaborations.

4.8 Coordination and Management of Connected Processes at Different Levels

Context: The overarching management of connected upstream and downstream processes within a company remains a key challenge and further improvements are expected to be enabled by digital technologies. Moving a step forward, the industry has started to be highly integrated, by connecting every single part of their value chain.[288] Furthermore, employing advanced digital technologies (IoT, cloud computing, big data, artificial intelligence and advanced data analytics) has created vast opportunities for cross-value chain synergies. The changes happen horizontally and cover the entire life cycle, from sourcing, to production and product distribution within a company. To support coordination of production within and across companies, process technologies will consequently require adaptation which could be supported by more reliable sensors, powerful algorithms, and advanced models linking process operations and plant logistics.

Coordination of processes and production will be applicable in and across a wide range of sectors, including the chemical-, biotechnological-, biorefining-, recycling-, water treatment/distribution sectors and other process industries. Coordination and management of processes, plants and sites will also be highly relevant to integrate a dynamic exchange of material and energy flows between municipalities and industry.

Market, overall expected impact: Integration of control, scheduling, planning and demand-side management will lead to efficient management of plants that are tightly connected by streams of energy and material flows but are owned by different companies, including scenarios on how to share advantages based on reliable models. Efficient coordination of interconnected process and plant networks will be crucial to deliver a real step-change towards higher energy and resource efficiency and will contribute towards a more circular economy, creating synergies beyond plant- site- and/or sectorial boundaries. These synergies will enable processes to adapt as flexibly as possible to fluctuations in the supply of raw materials and energy. Furthermore, coordinated delocalised production will facilitate the integration of customer and/or consumer data with production, increasing productivity, allowing for personalised products and enable new business models.

Digitally-enabled coordination and management of processes/plants/sites to connected value chains and industrial symbiosis will address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Next generation internet' 4.6, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and Industrial facilities in energy transition' (5.4), 'Agriculture, Forestry and the rural areas' (6.3), 'Seas, Oceans and inland waters' (6.4), 'Bio-based innovation systems in the EU Bioeconomy' (6.6), 'Circular Systems' (6.7), and 'Cybersecurity' (3.3), mainly via:

- **Improved collaboration and communication across the different stakeholders within value chains** by integrating raw material providers, producers and customers, which can for example connect feedstock suppliers in rural areas with biorefineries;
- **Managing production processes** to **use excess energy and waste from industrial processes within another industry through industrial symbiosis**, thereby enabling **circular operations**;
- **Significant efficiency improvements and cost reductions** can be achieved through demand and supply forecasting to enable responsive process scheduling;
- Use of **models applicable to process/plant coordination within and between companies** but also **across value chains** will create critical challenges and opportunities for **computing, next generation connectivity, data management and cybersecurity capabilities**.

Horizontal challenges:

- Making processes, plants, sites and value chains more connected draws upon accessing and exchanging data and information, which entail privacy, security and data confidentiality issues that will have to be addressed;
- Sourcing standardised and reliable data to feed into multi-parametric coordination models of a very high level of complexity of operations.

SUSCHEM PILLARS – MULTI-KETS:

Digitally-enabled coordination and management of processes/plants/sites to connected value chains and industrial symbiosis is expected to have a strong horizontal impact on RD&I in **Advanced Process Technologies** (**Chapter 3**) and especially on processes related with the integration of waste as feedstock (feedstock fluctuation) and energy fluctuations: 'Tolerant and intensified reactors and Processes tolerant to feedstock variability (3.1.1)' or 'Energy fluctuation (3.1.2)' or 'Electricity fluctuation (3.1.3)' as well as 'Modular production (3.2)', 'Separation process technologies (3.3)', 'New reactor and process design utilising non-conventional energy forms (3.4)', 'Power to chemicals ', 'Industrial biotechnology/ bioprocess development (upstream & downstream (3.10.2)', 'Waste valorisation process technologies 3.11' and 'Process technologies for advanced water management 3.12'.

Within **Enabling Digital Technologies**, the relevant topics include: 'Cognitive plants: (real-time) process simulation, monitoring, control and optimisation 4.3', 'Process Analytical technologies (PAT) 4.2', 'Advanced data analytics and Artificial intelligence 4.4', 'Digital support of operators and human-process interfaces 4.6', 'Predictive maintenance 4.5', 'Data sharing platforms, data security 4.7' and 'Distributed ledger technologies 4.9'.

RD&I Actions

4.8.1 Coordination of processes within a company accounting for supply chain demands

Context: Through modelling of connected production processes within a company, improved planning and scheduling can be achieved. At the second level, the integration of the supply chain and market/customer demands can be optimised through responsive process scheduling to achieve efficiencies that reduce the overall carbon footprint of the final product. Finally, real-time transfer of product information enables use of resources with variable quality. Interaction with customers operations can provide real-time recommendations to optimise both own and customers' processes.

Specific challenges:

- Mixed optimisation of batch and semi-batch trajectories and production scheduling, addressing the trade-off between the maximisation of throughput, energy efficiency, waste minimisation and other sustainability goals;
- Integration of production and utility planning and scheduling of improved energy efficiency and minimisation of waste (waste and water management);
- Improved planning and management to optimise efficiency and reliability of supply in the presence of fluctuations of feedstock quality, cost and availability;
- Integration of procurement and predicted deliveries into the planning;
- Integration with electric-power procurement, adaptation to the supply of electric-power from renewables, demand-side management, energy data management, energy operations, feedback systems for energy resources;
- Integration of predictive maintenance with planning and scheduling.

4.8.2 Coordination of processes within a company for product customisation

Context: Digital technologies enable product customisation and delocalised production to meet specific consumer/end-user needs in applications such as personal care, food, or pharma. This can also include value chains that deliver just-in-time (JIT) products. Companies within the chemical and biotech sectors can thus develop differentiated value-based propositions for their customers and grow their portfolio of products and services.

Specific challenges:

- Complexity to remote control and schedule delocalised and/or modular production units;
- Product customisation has a large effect on process parameters optimisation, translating into a much higher complexity in process modelling, scheduling and dynamic control;
- Control of the final product quality, performance and safety over standardised procedures;
- Prosumer models new digitally enabled business models.

4.8.3 Coordination of processes across companies and industrial sectors

Context: Industrial symbiosis can be coordinated digitally to couple production under different ownership to maximise overall efficiencies. It includes integrated waste and energy management optimisation.

Specific challenges:

- Making different companies and sectors more connected implies accessing and exchanging real-time data, leading to privacy, security and data confidentiality challenges;
- Complexity of adoption across companies and/or sectors due to integration of large volumes and complexity of non-harmonised data to be processed;
- Alignment on business model criteria to share potential benefits and IP between the different actors.

IMPACT EXAMPLES:

Example 1: Mapping of potential industrial symbiosis streams (energy/materials) and activities based on a technical methodology to identify cross-sectorial symbiosis (chemical, cement, steel, minerals and engineering) using data-analytics/decision-making support derived from 'sector blueprints' to overcome confidentiality issues for industrial data exchange and availability.[289]

Example 2: 4 % reduction in GHG emissions, up to 10 % reduction of the use of energy from non-renewable sources, 25 % waste minimisation and 10 % reduction of fresh water consumption by developing methods and tools for coordinated process monitoring and optimal dynamic planning, scheduling and control of plants, industrial sites and clusters under dynamic market conditions.[290]

TRL(now) & TRL(2030): Technologies aiming at making industrial processes more connected as well as technologies for achieving real-time connected supply chains have achieved a TRL 2-4. More R&I and demonstration activities are recommended to develop suitable modelling capabilities and demonstrate the feasibility of implementation in the chemical sector by 2030.

4.9 Distributed-ledger Technologies

Context: Chemical companies nowadays need to ensure the integrity of their data input and output (e.g. 88 % of industry executives revealed that their organisations are using data at an unprecedented scale for critical and automated decision making).[291] It is equally important for chemical companies to have a system of control mechanisms that can provide greater assurance to all participating stakeholders across the supply chain. Distributed-ledger technologies (e.g. blockchain) are a decentralised, reliable, shareable and immutable ledger of all transactions across a network, including different geographies, multiple sites, and organisations. The relevance and efficacy of distributed-ledger technologies becomes applicable in areas such as transparency of supply chains (tracking and traceability) and research data exchange. In the context of transitioning to sustainable circular supply chains, such technologies enable tracking of materials and products along (many) lifecycles.[292] The beneficial adoption of such technologies brings promises for the development of a sustainable bioeconomy.

Market, overall expected impact: Distributed ledger technologies, such as blockchain, could result in €75 to €125 billion in growth for the European chemical industry[293], considering the total EU chemical industry sales of €540 billion.[294] Distributed ledger technologies have thus great potential to improve supply chains in a wide range of sectors: agri-food, chemicals, pharmaceuticals and medical products, or high-value goods[295] through assisting industrial symbiotic networks by enabling digital trust on sharing data related to transactions along value chains.

Distributed-ledger technologies address several **Horizon Europe (HEU) clusters and areas of intervention areas**: 'Cybersecurity' (3.3), 'Manufacturing technologies' (4.1), 'Key digital technologies' 4.2, 'Emerging enabling technologies' 4.3, 'Advanced Materials' 4.4, 'AI and robotics' 4.5, 'Advanced computing and big data' 4.7, 'Circular industries' 4.8, 'Low carbon and clean industries' 4.9, 'Buildings and Industrial facilities in energy transition' (5.4), 'Food systems' (6.5), 'Bio-based innovation systems in the EU Bioeconomy' (6.6) and 'Circular Systems' (6.7) by the following factors:

- **Increased transparency** for how products are processed across supply chains (from raw material origin to end-use), will allow producers to tailor processes to customers in addition to enabling the better management of resources as well as the transparent tracking of the circularity and safety of their products;[296]
- **Increased efficiency of transactions and automating manufacturing operations** by changing the way supply chains operate in a wide range of sectors, closely linked with the chemical sector, including food, pharma, refining (incl. biorefineries), and energy.

Horizontal challenges:
Digital-ledger technologies, being emerging and disruptive, present adoption and scalability challenges associated with:

- Standards development and alignment (e.g. how records are designed, what information is included or how the verification mechanisms work).[297] Hence, the chemical industry and its upstream and downstream partners across the supply chain need to agree and develop common standards. This includes standards for minimising energy consumption, given the current energy-intensity for implementation (e.g. energy-intensive cryptocurrency validation process);
- Digital-ledger technologies are based on accessing and exchanging data and information, which entail privacy, security and data confidentiality issues that will have to be addressed.

SUSCHEM PILLARS – MULTI-KETS:

The implementation of Digital-ledger technologies is expected to have a strong impact on **Advanced Materials (Chapter 2)** through enabling all the described aspects on circularity-by-design and on 'Bio-based chemicals and materials (2.3)'.

Distributed ledger technologies for the tracking of raw materials and the production footprint of the final chemical product will bring links and Advanced Process Technologies (Chapter 3), and especially related with the integration of waste as feedstock (feedstock fluctuation) including the following topics: 'Tolerant and intensified reactors and Processes tolerant to feedstock variability (3.1.1)', 'Catalysis (3.9)', 'Industrial biotechnology/ bioprocess development (biomass & waste valorisation with IB (3.10.3)', and 'Waste valorisation process technologies 3.11'.

Within **Enabling Digital Technologies**, the relevant topics include: 'Laboratory 4.0-Digital R&D (4.1)', 'Coordination and management of connected processes at different levels 4.8', and 'Data sharing platforms, data security 4.7'.

RD&I Actions

4.9.1 Enabling transparent supply chains

Context: Implementation of decentralised platforms using digital ledger technologies to track-and-trace products throughout supply chains. Blockchain technology has great potential to provide transparency and communication in global value chains. Their protocol enables trusted data exchange in fragmented supply chains without public disclosure of datasets or supply chain partners, therefore protecting a company's privacy and sensitive information. Achieving a standard for traceability to origin would enable the proof of origin of materials, therefore fostering recycling practices. Achieving traceability and transparency could highly benefit, for instance plastics supply chains, by involving all value chain partners, including suppliers, processors, manufacturers, and brand owners to choose traceable, sustainable and circular materials.

Specific challenges:

- Barriers pertaining to adopting digital ledger technologies in supply chains stem from technology immaturity, data security, energy intensity, regulatory uncertainty, and joint efforts across complex value chains;[298]
- Lack of successful implementation or high-impact use cases for these technologies in the chemical sector to date.

Specific expected impact: Improving traceability, transparency and control of data related to transactions along supply chains and enabling a circular economy, recycling processes and related new business models.

IMPACT EXAMPLES:

Example 1: Design of an open platform to encourage plastic reuse practices through a monetary system of PCoins and PWallets maintained by a blockchain-based architecture which will safeguard trusted plastics reuse transactions among citizens and inventors, boosting citizens awareness, circular economy practices, and sustainable innovation.[299]

Example 2: Development of a personalised full-service technology, based on IoT, AI and Blockchain,, to provide a personalised end-to-end trace and tracking service and transparency along the cold chain in fresh food products and pharmaceuticals, avoiding losses of €6,300 million in the food production and losses of €35,000 million for the pharma industry.[300]

Example 3: Development of a blockchain protocol that traces mineral supply chains worldwide (e.g. gold, tin, tantalum, tungsten or copper) from the point of extraction to the factory, allowing mines, processors, transporters and other stakeholders in the sector to enable responsible sourcing.[301]

TRL(now) & TRL(2030): Distributed ledger technologies for improving traceability, transparency and control of data related to transactions in other sectors (e.g. financial sector) have achieved a high technology readiness. It is critical to move towards use cases for demonstrating the feasibility of implementation in the chemical sector by 2030.

4.9.2 Enabling research data exchange – Open Science

Context: Research is often conducted through collaborative efforts between different stakeholders where the exchange of research data is required. Platforms using digital ledger technologies (e.g. fitchain) can be used to safely exchange (encrypted) data, ensuring transparency on the data ownership and further processing by researchers. This reduces innovation/ development time across the different steps of the pipeline and allows scientists to build on experimental design and train R&D models through open, yet controlled, access to data.

Specific challenges:

- Lack of successful implementation or high-impact use cases of these technologies in the chemical sector to date.

5 HORIZONTAL TOPICS

5.1 Sustainability Assessment Innovation

Context: Over the past decades, there have been fundamental **methodological advancements** in assessing sustainability. Major progress is found in adopting the life cycle perspective, mostly for assessing the environmental sustainability of products and services. Nonetheless, the evaluation of technologies at lower technology readiness levels needs to be improved to also enable early-stage sustainability-based decision making. Furthermore, multi-objective optimisation and sustainability assessment (both environmental and techno-economic) for products and processes would also contribute to a more informed decision making, considering different impact parameters. Extending science-based targets across impact categories, considering different spatiotemporal scales and sectors, is an additional factor for improving the quality of sustainability assessment output. Fundamental and applied research and innovation, as well as European standards for measuring progress in meeting these targets, are required to address these challenges and help moving towards a truly sustainable society.

Furthermore, enabling **access to quality data and the development of necessary tools** will be fundamental to address the current challenges of sustainability assessment, including in the context of circular economy. Data confidentiality and proprietary data sets remain as significant barriers, whereas the emergence of big data methods, underpinned by digital trading platforms, digital research platforms, and various statistical data sets are promising directions for innovation in the generation of sustainability data. Databases will be developed to get more insights across value chains (evidence and understanding). Modelling for prospective sustainability assessment will be crucial to allow for the integration of dynamic data to achieve assessment at different levels: technology, product, and society.

Building on education and skills, within larger and smaller organisations, is recommended amongst other **uptake measures** for sustainability assessment. Although many large organisations in the chemical sector have proactively engaged with incorporating sustainability assessment into their businesses, a challenge remains to address the large number of smaller organisations who have yet to incorporate these methods and tools (SMEs, start-ups). Improving the uptake of sustainability assessment requires not just technical innovation, but also how users interact with the tools, data and the interactive process of evaluating sustainability. Intervention is therefore required to include sustainability assessment in best-practices for decision making within smaller and larger organisations.

It is also crucial to create networks of support for SMEs and start-ups to incorporate sustainability assessment tools as added-value to business development from an environmental but also social and economic point of view.

Expected horizontal impact - Global and EU challenges
'Sustainability Assessment Innovation' is expected to contribute across all UN Sustainable Development Goals (SDGs). All technological innovation priorities, as outlined under Advanced Materials, Advanced Processes and enabling materials will have to be supported by sustainability assessment. Similarly, regarding links with Horizon Europe (HEU) pillars, there should be strong relevance across all clusters under Pillar 2 (Global Challenges and European Industrial Competitiveness).

5.1.1 Methodological advancement

5.1.1.1 Development of European standards for Sustainability Assessment

Context: Sustainability can be assessed in different ways, using various types of methods and tools from qualitative assessment to fully quantitative life cycle assessment (LCA). However, many tools are currently only focusing on selected aspects of sustainability (e.g. LCA focuses on the environmental domain of sustainability) and alignment across domains (social, economic and environmental) is currently lacking. Moreover, not only a single life cycle of a given product or service should be assessed, but multiple cycles should be addressed to enhance circular economy considerations. To facilitate a coherent assessment of sustainability aspects, across scales and sectors, the development of European standards for sustainability assessment has been identified as a priority. This would require harmonisation of: i) existing methods, ii) metrics and indicators, iii) system boundaries as well as iv) terminologies for methods, tools and indicators. Such work should build on existing guidelines and standards such as the global International Organization for Standardization (ISO) standards for LCA and the United Nations Environment Programme (UNEP)/ Society of Environmental Toxicology and Chemistry (SETAC) guidelines as well as the Product Environmental Footprint guidance.

Constraints: Complexity on alignment on standards across sectors and value chains at European level.

EXPECTED IMPACT:

Coherent standards at European level could also facilitate the development of a global methodology for sustainability assessment with a potential significant impact as a foundation for enabling related certification.

5.1.1.2 Multi-objective optimisation and sustainability assessment (product/process development)

Context: Several methods for multi-criteria decision making exist, yet their usability is based on the case and the scope of the assessment. In addition, there is a lack of standardised frameworks for multi-objective optimisation. The compatibility between existing frameworks for multi-objective optimisation with lifecycle assessment analysis (LCA) and techno-economic assessment (TEA) should be studied and improved, including the consistent integration of multiple environmental and techno-economic indicators. Currently, the compatibility between assessing environmental sustainability and assessing economic sustainability needs be improved, based on standardised data for both. Further guidelines are also required for weighting and evaluation of different sustainability aspects towards harmonised multi-objective optimisation.
More robust mathematical methods for multi-objective optimisation can be appropriate in sectors with well-developed process modelling frameworks. Multi-objective optimisation, using statistical models developed with the aid of 'big data' methods, could be appropriate in various sectors.

Constraints: Lack of standardised frameworks for multi-objective optimisation, access to (digitised) data and advanced statistical methods across industrial stakeholders.

EXPECTED IMPACT:

Decision support methodologies leading to more rational design and faster implementation of sustainable solutions with potential links to new business models.

5.1.1.3 Extending science-based targets across impact categories

Context: Currently, the evaluation of environmental sustainability focuses on relative improvements. Emissions into the environment and extraction of any resources from the environment, however, are restricted by the biophysical conditions of our sustaining Earth system. Targets for impact categories that consider these conditions/limitations would lead to effective improvements, beyond increasing efficiency and would allow to measure real progress in relation to such defined targets. Current targets are not able to properly relate to actual biophysical conditions, beyond GHG emissions.
Among the most important priorities is to define science-based human and ecological health targets, accounting for the multitude of chemicals produced and the relevant human and environmental exposure, spatiotemporal variability and the different relevant scales. To achieve such an ambitious goal, multi-disciplinary research will be necessary but also engagement and involvement across stakeholders, including the industry and public stakeholders.

Constraints: Spatial granularity challenges, co-exposure/mixtures of chemicals, variable targets from local to global scale.

EXPECTED IMPACT:

Target setting, and progress measurement, aligned with actual biophysical targets across impact categories, will provide a quantitative dimension for assessing the sustainable development at societal and industrial levels, which is currently more challenging based on indicators reflecting relative improvements. Additionally, integrating impact categories relevant to human and environmental health could be an important enabler for 'safe-by-design' for chemicals and materials along their lifecycle.

5.1.1.4 Methodologies for ex-ante LCA (qualitative and semi-quantitative assessment)

Context: Most sustainability assessment results currently focus on fully developed and marketed products and services. However, more influence on choices of materials, chemicals, resources, and processes can already be made at design and early technology stages, while related data are currently widely missing. Extrapolation and upscaling methods and factors are urgently required to address this gap, allowing for sustainability considerations at early design and development stages. Methods for improved ex-ante sustainability assessments are urgently required to facilitate early-stage evaluations that usually come with limited data availability about the studied product or service.
Various options should be flexibly evaluated to identify sustainable solutions, based on, for example, prognostic modelling to assess possible future scenarios. Case

studies on ex-ante LCA, applicable to emerging technologies, could start from mining available data and sustainability assessment results to derive generalisable rules for early-stage assessment and upscaling. The uncertainty, inherent to any ex-ante assessment, should be carefully managed as well as the communication of any related results.

Constraints: Large variability in technologies, scenarios and options to find generalisable pathways for early-stage assessments.

EXPECTED IMPACT:

Facilitate decision making and, if successful, this could also have a much wider impact on entire sectors and supply chains than doing any LCA or similar assessment at higher TRLs.

5.1.2 Sustainability Assessment innovation –data & tools

5.1.2.1 Data sharing platforms across value chains

Context: Sustainability assessment has been hampered by the lack of good quality and accurate data on production processes and supply chains. Current technological trends and advances on digital technologies for data collection and data sharing offer a unique opportunity to achieve substantial improvement against these challenges. To this aim, development of data sharing platforms for data sharing across value chains would make sustainability assessment easier and get better quality results. However, important points to be addressed are: data access, ownership and barriers of confidentiality. Moreover, data standardisation of data representation, using either categorical or ontological frameworks, is an important milestone as data are currently unstructured. Data sharing platforms could also represent new business opportunities, for instance for SMEs and overall enabling sharing practices across the innovation ecosystem. Availability of standardised datasets can enable the development of new assessment and innovation tools, such as the large-scale use of digital twins and evolutionary algorithms for scenario evaluation for large interacting systems, such as regional-scale circular economy models.

Constraints: Data confidentiality is a key constraint; setting up of a framework for collecting data and further aggregating them before sharing, without compromising on accuracy and granularity, should be investigated.

EXPECTED IMPACT:

Increase the reliability of sustainability assessment, facilitate SMEs to integrate sustainability assessment in their decision making, reduce time and resource intensity for sustainability assessment across value chain stakeholders.

5.1.2.2 Tools for prospective sustainability assessment

Context: Sustainability assessment of new processes and products is most often performed at technology level only, without a proper consideration of future upscale of the technology, its market penetration and the overall impact of technology adoption at full market scale and in different geographical locations. At best, ad-hoc extrapolation in simple "expert option-based" scenarios are performed to this aim. However, assessing the future impact of a technology at full market scale is very much needed to monitor and steer technology development in relation to and against sustainability development objectives. Current LCA-based methods rely on static datasets which can be used to some extent for prospective evaluations, depending on the definition of the scope of the assessment. The limitations of LCA-based datasets lie under their variable quality and frequency of updating. Tools are needed to enable sustainability assessment simulations and research could build on current digital innovation trends such as artificial intelligence (AI) and machine learning techniques. It is also imperative to develop new approaches that are based on innovations in data science. The latter includes ontological and categorical representations of data that would allow algorithmic assembly of datasets and linking of models across multiple domains of technologies, as well as AI-based methods for assembly of life cycle inventories and optimisation and exploring future scenarios over multiple time and spatial scales.
Prospective sustainability assessment, fuelled by value chain assessment, prospective modelling of technology adoptions and consequential sustainability modelling will offer a pertinent framework to derive consistent extrapolations across the different sectors. This will in turn lead to minimising overlaps, double counting and eventually provide a more accurate estimation of the impacts of R&D projects. A possible priority focus could be the circular economy.

Constraints: A key constraint is the availability of data for: i) the upscale of technologies, ii) evaluating secondary and tertiary aspects effects of technology adoptions, and iii) the usability of the developed framework and tools by professionals because of their complexity.

EXPECTED IMPACT:

Achieve harmonised approaches for prospective sustainability assessment at different levels: Technology, product, and society. Perform more comprehensive, consistent and transparent assessment as compared to current best practices.

5.1.2.3 Data analysis for better understanding of feedstock variability: enabling Circular Economy

Context: The progressive implementation of circular economy solutions in value chains involves a relative high variability in feedstock composition (especially for biomass and plastics waste). Therefore, understanding such variability is key for reaching circularity objectives, given the impact of feedstock on the end product quality, process metrics and overall environmental footprint. Leveraging the current trends in data and analytics, including big data to handle large datasets but also digital technologies for advanced modelling should allow for:

- Access to and processing of data on feedstock flows across value chains and eventually simulations of material flows;
- Chemical and/or biotech processes optimisation;
- Improving product properties and sustainability profile.

The final purpose is to develop tools enabling circular economy and ensuring the sustainability profile of related processes and products, utilising data from across all value chain partners.

Constraints: Access to data, capability to account for very complex variations of composition (e.g. seasonality, geographical, and value chain variations) especially when it comes to waste, which includes secondary biomass, plastics waste and municipal waste.

EXPECTED IMPACT:

Sustainability assessment tools, accounting for feedstock variability effects, will enable a sustainable Circular Economy by supporting decision making and innovation which includes informed optimisation in product and process design and business models development.

5.1.3 Sustainability Assessment innovation – uptake

Further developments in uptake of sustainability assessment are essential to:

- Explain to all stakeholders why change is needed, and enable mindset change in society;
- Support decisions by policy makers and private stakeholders;
- Ensure best/most appropriate assessment methods and tools are used.

To ensure greater uptake of sustainability assessment approaches broadly across the chemicals sector and value chains, the following actions are proposed.

5.1.3.1 Framework for recommended methodologies and structures on early-stage and semi-quantitative assessments

Context: This action calls for the development of a framework to demonstrate a best-practice structure for an early-stage and semi-quantitative sustainability assessment toolkit, incorporating environmental, economic and social factors. The framework should consider best-practice user-interface specifications (e.g. data traceability, visualisation), in addition to sustainability indicator calculations.

See also: Methodologies for ex-ante LCA (qualitative and semi-quantitative assessment)* *(5.1.1.4)***

Constraints: Requires consensus building through EU level experts and sector groups.

EXPECTED IMPACT:

The toolkit framework should allow in-house industry, commercial and public sector tool developers to improve existing and new tools for early-stage sustainability assessment and decision making, leading to more consistent approaches through value chains.

5.1.3.2 Development and maintenance of an Open Access sustainability screening toolkit

Context: Development of an Open Access version of the action **5.1.3.1** framework (above) would allow a broader range of organisations, who currently lack their own in-house tools, to integrate sustainability evaluations into day-to-day operations. The toolkit would also allow organisations to improve, integrate and adapt their own in-house tools to get greater consistency through value chains.

** See also 'Sustainability Assessment innovation –data & tools* ***(5.1.2)***

Constraints: Toolkit to be free or low fee access; to be supported beyond its initial development to allow longer term maintenance and support for users.

EXPECTED IMPACT:

Greater uptake of sustainability assessment, in particular by SMEs and start-ups.

5.1.3.3 Coaching programmes on sustainability assessment for SMEs

Context: Although many large companies have incorporated sustainability assessment into their operations and projects, many more organisations, particularly SMEs, are new to sustainability assessment and do not use any sustainability information whilst running improvements on projects or designing new products and processes. This action calls for a programme to actively coach these organisations to use screening and semi-quantitative toolkits (see **5.1.3.1**), demonstrating how they can help their businesses to use sustainability evaluations to improve decision making. Actions to achieve this can include: development of a consistent set of assessment data frameworks, secure data sharing platforms, and tools applicable to the various SME contexts, whilst allowing for an active communication among various SMEs. Training material and open-access assessment platforms (see **5.1.3.2**) with easy-to-use and adaptable user interfaces would be enablers for supporting SMEs towards the broader uptake of sustainability assessment.

Constraints: Diversity of application contexts and related assessment/data requirements; dependencies on supply chain information; need for numerous targeted and tailored assessment programmes.

EXPECTED IMPACT:

Much wider application of sustainability assessment and related decisions on product design and development across sectors; broader awareness and implementation of sustainability-based solutions in SMEs.

5.1.3.4 Definition of a minimum set of common categories and indicators for assessment

Context: Guidance is required for multi-criteria assessment at European level through the definition of a minimum set of common categories and indicators to be considered for reliable sustainability evaluations.

Constraints: Complexity of revision/ update at EU level; risk of limited data availability on chosen common categories and indicators.

EXPECTED IMPACT:

Improve consistency and communication on sustainability evaluation for technology assessment and policy design.

5.1.3.5 Education on sustainability assessment at all levels of education and types of curricula

Context: The principles of sustainability should be implicitly imbedded in education at all levels and emphasise system-level thinking and numerical methods in higher education. Specifically, sustainability should be included in engineering and natural sciences undergraduate degrees as a compulsory topic, with inclusion of such topics as ecology, climate, energy, water and food, with inclusion of Sustainable Chemistry and 'clean' technologies, metrics of sustainability assessment, including LCA, techno-economic analysis, multi-criteria decision making, analysis of complex interacting systems (for engineers), and supply-chain level sustainability analysis (for engineers and manufacturing). This training can be effectively accompanied by digital skills, advanced modelling and AI.

Constraints: Complexity and breadth of topics under sustainability assessment; integration within existing curricula might be challenging.

EXPECTED IMPACT:

Increased awareness on sustainability and sustainability assessment; improved decision making, including industry but also consumers.

* See also 'Building on Education and Skills Capacity' in Europe 5.3

5.2 Safe-by-design for Chemicals and Materials

Context: In view of a rising worldwide population and economic growth, there is an increasing volume of chemicals and chemical-intensive products. This enhances the need to ensure the sustainable use of natural resources but also the safety and overall sustainability of chemicals, materials, products and markets, especially under the global transition to circular economy. Under this context, the chemical industry is also working on improvements in a range of areas, including Health, Safety and Environment (HS&E), and promoting the safe management of chemicals in the supply chain and throughout their lifecycle.[302] At the same time societal concerns[303] on the impact of chemicals on human and environmental health persist. As underlined in a recent recommendation paper containing 'safe-by-design' innovation priorities for Horizon Europe,[304] the concept of 'safe-by-design' aims to prevent negative impacts on the environment and human health, considering safety aspects early in the design process of chemicals, materials and products. It therefore provides an innovation opportunity for existing and novel applications at EU level. The 'mid-century' vision of the European chemical industry also embraces the substitution of problematic substances as an innovation opportunity and it underlines the continuous support for objective criteria, tools and methodologies to avoid 'regrettable substitution'.[305]

Placing more emphasis on innovation for 'safe-by-design' aims to prevent risks. Moreover, it is an enabler for the transition towards circular economy, which benefits from inherently safer materials that maintain their quality through multiple cycles, including repair, reuse and recycling. Essential elements and objectives of 'safe-by-design' include:[306]

- **A functional approach for safe-by-design**, accounting for innovation that starts from considering the desired function(s) provided by a substance within a product to innovate from molecular level to higher levels: Materials, products, processes and business models;
- **Minimising toxicity and combine with overall sustainability improvements (full lifecycle perspective)**: The starting point of 'safe-by-design' is to minimise toxicity (including persistency, bioaccumulation, and products of incomplete degradation/mineralisation). Safety is also broader than chemical toxicity, including microbiological safety and biosafety, when expanding to biotech. Nonetheless, global challenges related to climate change, environmental degradation and social sustainability can only be tackled with products that are sustainable in a wider sense, including aspects beyond safety, such as energy and resource efficiency, emissions and exposure minimisation. Overall, 'safe-by-design' requires a full life cycle perspective and needs to be combined with overall sustainability improvements, also to avoid the shifting of negative consequences across life cycle stages and impact categories;
- **Innovation as a multidisciplinary approach**: going beyond drop-in replacements and towards 'safe-by-design' implies systemic thinking and the involvement of various disciplines: e.g. chemistry, biology, toxicology, sustainability assessment, product, materials and process design, extending to supply chain management, data management and the integration of enabling digital technologies which will also not only enable innovation (e.g. materials modelling and design) but also provide transparency in value chains;
- **An integrated and collaborative network**: 'safe-by-design' encompasses cross-value chain collaborations and communication amongst different stakeholders: from chemicals and materials producers, to brand owners and end-users. Furthermore, innovation will require the contribution of the full innovation ecosystem and knowledge sharing can also become beneficial across sectors.

Overall, 'safe-by-design' is a concept that is in line with Sustainable Chemistry, with the potential of becoming an innovation opportunity. It is also an opportunity for the EU to take the lead in the circular economy transition by developing innovative, safe and sustainable materials, chemicals, products and services for new or existing applications.

EXPECTED IMPACT: GLOBAL AND EU CHALLENGES

'Safe-by-design' innovation would contribute to many, if not most, of the UN Sustainable Development Goals (SDGs) and is relevant for the achievement of much of the 2030 Agenda for Sustainable Development. Some of the most relevant SDGs include: sustainable agriculture (SDG 2); healthy lives and well-being (SDG 3); clean water and sanitation (SDG 6); decent work and economic growth (SDG 8); resilient infrastructure, inclusive and sustainable industrialisation and innovation (SDG 9); responsible consumption and production (SDG 12); life below water (SDG 14) and life on land (SDG 15).

'Safe-by-design' and its links with Horizon Europe (HEU) pillars, and possibly other European programmes (e.g. LIFE), has potential links and opportunities in Pillar 2 (Global Challenges and European Industrial Competitiveness), in particular the clusters: 'Health' (1), 'Digital, Industry and Space' (4) and 'Food, Bio-economy, Natural Resources, Agriculture and Environment' (6).

5.2.1 Focus action areas for 'safe-by-design': Addressing RD&I and further enabling actions

To achieve the above-stated objectives, three areas of action are being highlighted:

i. **Thematic research, development and innovation** that could be driven by **functionality** relevant to: **Materials, formulations and industrial processes**;

ii. **Methodological development or improvement** for any (re)design of chemicals and materials, minimising toxicity and combining with overall sustainability improvements (integration of circularity);

iii. **Creating an enabling environment that includes knowledge development, networks formation and education** to give focus to RD&I actions but also imbed them in a wider strategy.

RD&I should allow technical challenges for 'safe-by-design' to be overcome that would be applicable to functionalities in materials, formulations and industrial processes, especially in problematic areas where it has been difficult to find safer alternatives with equivalent performance. Such RD&I can focus on the function performed by chemicals (e.g. repellence) rather than meeting the chemical structure of additives. Innovating on material structures, product and process improvements can thereby be given more emphasis. Building on the Safe Chemicals Innovation Agenda,[307] and further consultation, which also included SusChem stakeholders, a non-paper with Horizon Europe innovation recommendations was produced. **Table 7**[308] indicates a list of functions for consideration under RD&I. This list is not exhaustive, but it covers critical functions provided by industrially applied chemicals that are relevant to materials, formulations and processes. Stakeholders also highlighted circular economy and feedstock variability as factors increasing the innovation complexity and underlined the links with parallel advances on waste treatment as well as separation/ purification technologies. Additional challenges include complex performance implications and cost effects (application-dependent), and changes across values chains. RD&I on 'safe-by-design' should also consider all sustainability aspects to not compromise any significant parameter upon changes at chemical structure or material composition level. Such a broader innovation perspective is thereby recommended to be complemented by methodological development (**Table 8**)[309] but also the involvement of multiple disciplines and stakeholders across value chains (**Table 9**).[310]

Table 7: RD&I Actions: Addressing Thematic Research, Development and Innovation (Functional Approach)

MATERIALS	
WATER, GREASE AND DIRT REPELLENCE	• New materials design approaches to achieve inherent repellence performance. • Innovative repellent materials, using alternative chemicals with positive scores on safety and ability to mineralise.
FIRE SAFETY	• Innovative materials with inherently flame-resistant function. • Materials design to reduce additive exposure/leaching to the environment (intermediate solution).
PLASTICISING	• Innovative materials with the same functionality (flexibility, durability) in the absence of hazardous additives (in final product and production process). • Novel, safe and sustainable material/alternative chemical combinations with plasticising functions.
FORMULATIONS	
PRESERVATION	• Preservation systems based on alternative mechanisms (*e.g. combination of physical & chemical treatment*), maintaining shelf life and biosafety. • Mechanisms of antimicrobial activity with new chemical-material combinations (raw materials combinations/ synergistic effects and design approaches) with an increased specificity for target organisms.
FUNCTIONS PROVIDED BY SURFACTANTS	• Sustainable production of alternative surfactants, combining safety and life cycle sustainability performance, accounting for feedstock impact and especially further considering biodegradability according to standards. • Rational formulation (re)design, understanding the behaviour of new/alternative surfactants in complex mixtures/formulations and their implications on product performance and scaling up production.
PROCESSES	
PROCESS FUNCTIONS PROVIDED BY SOLVENTS	• Innovative materials (*e.g. biomimicry and stimuli-responsive materials*) with reduced surface treatment requirements. This option brings challenges to overcome beyond material performance, extending to effects on process flexibility whereas the impact on material circularity must also be considered. • Process innovation to avoid and reduce the volumes of hazardous solvents in production. This could include process intensification or completely novel processing routes. • Alternative formulations/chemicals for process solvents (e.g. bio-based alternatives) upon thorough screening of their respective sustainability and safety profiles.
PROCESS REGULATION	• Relevance to chemical curing: inherently strong and versatile polymers - innovative foams and resins, tackling cost and scalability challenges.
SURFACE PROTECTION	• Alternative materials (*e.g. polymer engineering, nanotopography*) that are inherently resistant to corrosion or fouling. • Development of new techniques for surface treatment (e.g. metal surface treatment processes alternatives (e.g., vapour deposition. ultrasonic or UV techniques).

Additional functionalities for consideration: **Materials: UV-stabilisation and anti-oxidants; **Formulations**: stabilisation, colorants, mechanical abrasives and include solid mixtures/ formulations; **Processes**: preservation for process fluids, additives and fuels.*

*** Relevance to **Materials** and **formulations design**: Microplastics could refer to the undesired release and accumulation of particles into the environment. Hereby, the release might be a consequence of intentionally added microplastics or resulting from use during the product lifecycle (use phase and end-of-life) (i.e. wear and degradation).*

'Safe-by-design' builds on existing risk assessment and management frameworks for which data and tools exist and are under continuous improvement. To make sure that chemical substances can be produced and handled safely, adequate knowledge about their properties has been a prerequisite. A major part of product safety data is derived from toxicological and eco-toxicological studies. Based on the "Three Rs Concept", every new methodology that results in an enhancement of animal welfare is an alternative method. This can be achieved either by 'R'eduction of the number of laboratory animals used, 'R'efinement of the test procedure, or by 'R'eplacement of animal tests by in vitro and in silico methods. The development and use of alternative or new approach methods to reduce the number of animals in product safety testing is a continuous innovation task. Within the context of new product development, 'safety-by-design' has gained attention as well as progress by the development of in vitro methods. These methods are meant to allow for screening of many new compounds during early stages of development and the selection of those candidates which demonstrate a low hazard profile. Moreover, the possibility to generate a high amount of test results within a reasonable short period of time facilitates the development of classical or artificial intelligence-based computer models that link chemical structures with biological outcome (structure-activity relationship). Such information can be used immediately by scientists in the process of new product development – providing essential early information for the safety by design concept. Finally, new approach methods jointly provide a better insight into the molecular mechanism or mode of action, resulting in toxicity.

Regarding existing risk assessment and risk management frameworks, they answer to very specific questions and purposes, ranging from qualitative, semi-quantitative to quantitative approaches applied for chemical safety assessment, product life cycle assessment, cost-benefit analysis, high-throughput risk screening and prioritisation, and alternatives assessment.[311] Further adaptation to address more complex questions but also account for the transition to circular economy as well as the overall weighting and assessment of the sustainability profile of any alternative solutions are recommended (links with 'Sustainability assessment innovation' 5.1). The more specific priorities regarding methodological development are outlined in **Table 8**, suggesting research and stakeholders' consensus on efforts/actions.

Table 8: RD&I Actions and Beyond: Methodological Development or improvement: 'Safe-by-design'

CRITERIA AND TARGETS	• Harmonised and validated criteria and science-based targets for safety and broader sustainability for the full life cycle of chemical/material/product/service, also addressing circularity; • Criteria, targets and methods applicability early in the (re)design process of chemicals and materials, ensuring consistency in evaluation and early stage prioritisation.
EFFICIENT 'PREVENTIVE' TOXICOLOGY AND LIFE CYCLE TOOLS	• Efficient/flexible digital tools for integrating knowledge of toxicity into early design to evaluate safety impact ('Preventive' vs. 'predictive' toxicology); • Allow for more complex assessment via multiparametric toxicity but also LCA models (integration of risk assessment, LCA methodologies and circular design).
ACCESSIBLE DATA	• Make data available for designers [criteria for Findable, Accessible, Interoperable and Reusable (FAIR) data, open access databases)]; • Development of transparent, efficient and reliable methods to allow information transfer along supply chains (data sharing platforms).
STANDARDISATION	• Involve standardisation bodies to ensure optimum use of standards and development of new standards (data, methods, tools).

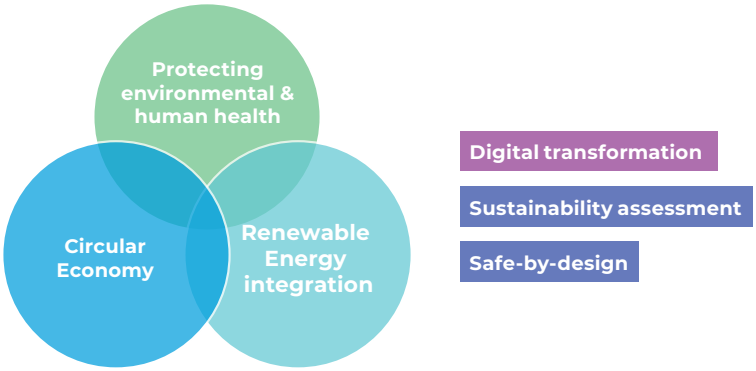
'Safe-by-design', as a new interdisciplinary approach, will need to be part of a wider strategy. In addition to RD&I efforts, and methodological development, creating an enabling environment is suggested. Knowledge exchange can be cross-sectorial and between larger industry and SMEs/start-ups. Under the horizontal topic of education/skills development (links with 'Building on education and skills capacity in Europe' 5.3), the relevant focus on developing necessary to 'safe-by-design' skills is also presented. Moreover, supply chain cooperation and coordination are additional essential aspects (**Table 9**).

Table 9: Creating an enabling environment for 'safe-by-design'

KNOWLEDGE DEVELOPMENT, NETWORKS AND EDUCATION	• Landscape analysis of existing disciplines, networks and organisations; • Network building as an objective or condition in funded projects; • Higher education, workshops, challenges and competitions, bootcamps, educational networks as start of a process of internalising safe-by-design in education and skills development.
SUPPLY CHAIN COOPERATION AND COORDINATION	• Scoping phase with stakeholders before technical research to: - Analyse context of the innovation (potential barriers); - Identify user needs and performance criteria; - Identify appropriate levels of research (materials, processes, products, chemicals); • Data and knowledge sharing platforms across value chains and different sectors.

5.3 Building on Education and Skills Capacity in Europe

Context: Addressing global challenges such as climate change, protecting human and environmental health, natural resource scarcity, industrial competitiveness and technological excellence, drives continuous efforts in research, development and innovation. It also fuels the urgency to develop education and training for highly skilled scientists and engineers in the chemical sector, securing expertise in emerging technologies and future socioeconomic realities for the challenges of 2030 and beyond.



Industrial Biotech | Sustainable Chemistry | Sustainable technology – Chemical Engineering

Innovation Ecosystem: Large Industry, Academia, SMEs, startups
National governments

Complex landscape: Multiple stakeholders at a national and EU levels

The transition to a Circular Economy, including the valorisation of alternative carbon feedstock and sectors coupling via integrated renewable energy systems, leads to drastic changes in the type of products and services that chemists and chemical engineers (will) provide, also making these fields increasingly interdisciplinary.[312] Moreover, under the fast-paced evolution of the chemical and biotech sectors, coupled with the digital transformation: manufacturing, supply chain and business models have changed. New value chains have emerged, as well as a growing demand for personalised products and a rising entrepreneurial culture in Chemistry, biotech and Chemical Engineering.[313,314,315] These developments have also induced changes in methodologies and tools used at R&D and production levels, resulting in new requirements for education and capacity development.

The core skills in Sustainable Chemistry, Sustainable technology/Chemical Engineering and Industrial Biotechnology will thus expand to areas such as digital skills, sustainability assessment, process design in the context of energy transition and materials circularity as well as safe-by-design, making the definition of the core skills and knowledge broader and more complex than today.

To address the above challenges, we need to enhance and further strengthen collaborations between academia and industry to foster an education and training landscape. This will enable us to meet the demand for future skills and prepares Chemists, Chemical Engineers and Biotechnologists with a combination of hard/technical skills but also professional competencies (see **Table 10**). Additionally, large companies can play an important role in enabling skills development by supporting dynamic cooperation with SMEs and start-ups. Learning aims and curricula are currently set at institutional or national level, yet this process could increasingly be shaped by activities such as international summer schools, workshops, bootcamps, challenges and competitions, fellowships, international educational networks, and post-doc research, but also hubs and through integrating the development of learning resources in research and innovation actions (RIAs/IAs) based on the innovation outcome of certain projects (*e.g.* **'SusChem Educate-to-innovate concept'**, *SPIRE 2016-2017 WP*).

Table 10: Cutting-edge skills for European chemicals innovation.

Core technical knowledge Examples	Wider technical knowledge Examples	Professional competencies Examples
Chemistry **Materials science** **Biology** **Biotechnology** **Physics** **Mathematics& Statistics** **Engineering (chemical-, bio-, mechanical-, electronic- etc.)**	**Sustainability** (e.g. LCA, toxicology, safe-by-design, circular design, ethics **Data and Digital skills** (e.g. machine learning, data science, big data, distributed ledger technologies, AI, computational modelling (materials& process levels), programming, robotics, cybersecurity, advanced measurement instruments and sensor networks, neural networks and deep learning) **Other areas:** Regulation (e.g. REACH), techno-economic evaluation, energy systems, Industrial symbiosis, risk assessment Intellectual property (IP)	Teamwork and building effective teams Collaboration Negotiation Interdisciplinary working Openness to change Diplomacy Multi-cultural sensitivity Decision-making Effective communication Influencing Leadership Diversity and gender balance values Entrepreneurship Critical thinking Curiosity Initiative Strategic thinking Commercial awareness/acumen innovation & business Project management

Examples of potential links with Horizon Europe (HEU) & other EU programmes/priorities:

- **ERASMUS+**
- **HEU – EU projects (integration of development of learning resources in RIAs/IAs), Marie-Curie mobility actions**
- **Digital Europe**
- **KICs (Knowledge and Innovation Communities) within the EIT (European Institute of Innovation & Technology)**
- **Open Science & Plan S**
- **ERC Synergy**

EXPECTED IMPACT – GLOBAL & EU CHALLENGES

The European Commission highlights that the investment in "education, science, technology, research, innovation and digitalisation is a prerequisite for achieving a sustainable EU economy" that meets the UN SDGS.[316] Also, Horizon Europe (HEU) regards education and training as important for the development of high value skills, productivity and growth as well as fostering the EU digital transformation (e.g. 'Cluster 2/ Culture, creativity and inclusive society' - 'Social and economic transformations (**2.3**)').

A digital transformation of process industries will result in increased productivity; more sustainable operations and greater agility of processes and their supply chains, in response to society's and their demands for high performance products, personalised products and transparency. Without a digital transformation of the chemical sector, circular economy models will be more challenging to achieve.

Supporting networks of digital innovation, between the large industry, academia, start-ups and SMEs, are needed to accelerate the required skills transformation within the chemical sector.

5.3.1 Education and Sustainable Chemistry: interdisciplinarity is key

The Need

Chemistry enables a plethora of sectors of our economy, from food, health and consumer care, housing and mobility to energy and clean water. The chemicals sector and downstream industries produce the building blocks for the products used in these sectors, thereby providing the material basis for the functioning of our society. At the same time, chemical production and the use of chemical products are associated with the extraction of resources, the consumption of water and energy and the release of a growing number of chemical entities into the environment. Due to this central role of chemistry for the material domain, it is essential to view it as integral for the system of sustainability and recognise its role for enabling sustainable development. The increasing importance of topics such as sustainability assessment and safe-by-design in the transition to a circular and more sustainable economy demonstrate a strong need for interdisciplinary research and skills development in areas that have not been part of 'traditional' Chemistry and Chemical Engineering curricula.

State-of-the-art

In higher education, the breadth of curricular content is managed by the compartmentalisation of Chemistry and its interactions with Chemical Engineering and Materials science. The field of Green Chemistry is described as "the utilisation of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacturing and application of chemical products". Green Chemistry and its principles have been increasingly introduced into higher education worldwide, albeit still being fragmented.[317] The programmes show enhanced emphasis on less waste, less energy and less toxicity for synthesis and related products, such as guidelines for the selection of less toxic solvents,[318] the use of renewable feedstock for synthesis,[319] catalysis,[320] or the development of materials for renewable energy.[321] With this, they have constituted an important transition in chemistry education and trained chemists to reduce pollution and improve on resource and energy consumption during chemical production. So far, however, these programmes do not address overarching topics in the context of sustainability. For instance, chemists and chemical engineers should also receive training in basic concepts of toxicology, ecotoxicology and environmental chemistry to create consciousness of 'end-of-life' issues. Similarly, the principles of safe-by-design, 'design-for-degradation', 'design-for-circularity' for targeted applications, are crucial for decreasing the persistence of chemicals in the environment but are rarely addressed in the respective curricula. Additionally, training on holistic sustainability assessment and the concepts of circular economy should be further emphasised.

The concept of Sustainable Chemistry has been emerging as a guiding principle to view chemistry in the context of sustainability given its profound impact on sustainable development. Understanding and applying chemistry in alignment with sustainable development requires education programmes that extend beyond the focus of green synthesis and train graduates to imbed core chemistry knowledge into sustainability system thinking.

Future needs – outlook

Programmes, from higher education to vocational training, should shift from the prevailing sub-disciplinary character of chemistry programmes to interdisciplinary ones, including for example: sustainability ethics and sustainability assessment metrics (e.g. LCA), techno-economic analysis, and multi-criteria decision making. Further skills should include, for instance, knowledge of relevant policies and regulations, a better understanding of toxicology and environmental health sciences, innovation management, alternative business models and change management. Especially for complex concepts, such as circular economy and safe-by-design, knowledge development, networks and education significantly require this kind of interdisciplinary approach (see **Table 10 above**).

Introducing this kind of interdisciplinarity without compromising on an adequate level of core chemistry knowledge is challenging. However, encouraging examples exist alongside a conventional chemistry curriculum, professional programmes, education hubs, and bootcamps for continuous professional development.[322]

5.3.2 Digital Skills

The Need

The digital transformation of the chemical industry will require building on competence in designing, performing and implementing digital technologies. Moreover, 'Industry 5.0' is expected to merge the high-speed accuracy of industrial automation with the cognitive, critical thinking skills of humans'. Data Science and robotic experimental platforms will become enablers alongside conventional R&D, modelling and the tools of Process Systems Engineering. Digitalisation also offers access to 'digital twins' and AI-driven simulation environments. However, to make the most of the digital revolution it will be essential to merge conventional skills and knowledge of chemistry, materials and processes with the emerging capabilities of digital technologies.

State-of-the-Art

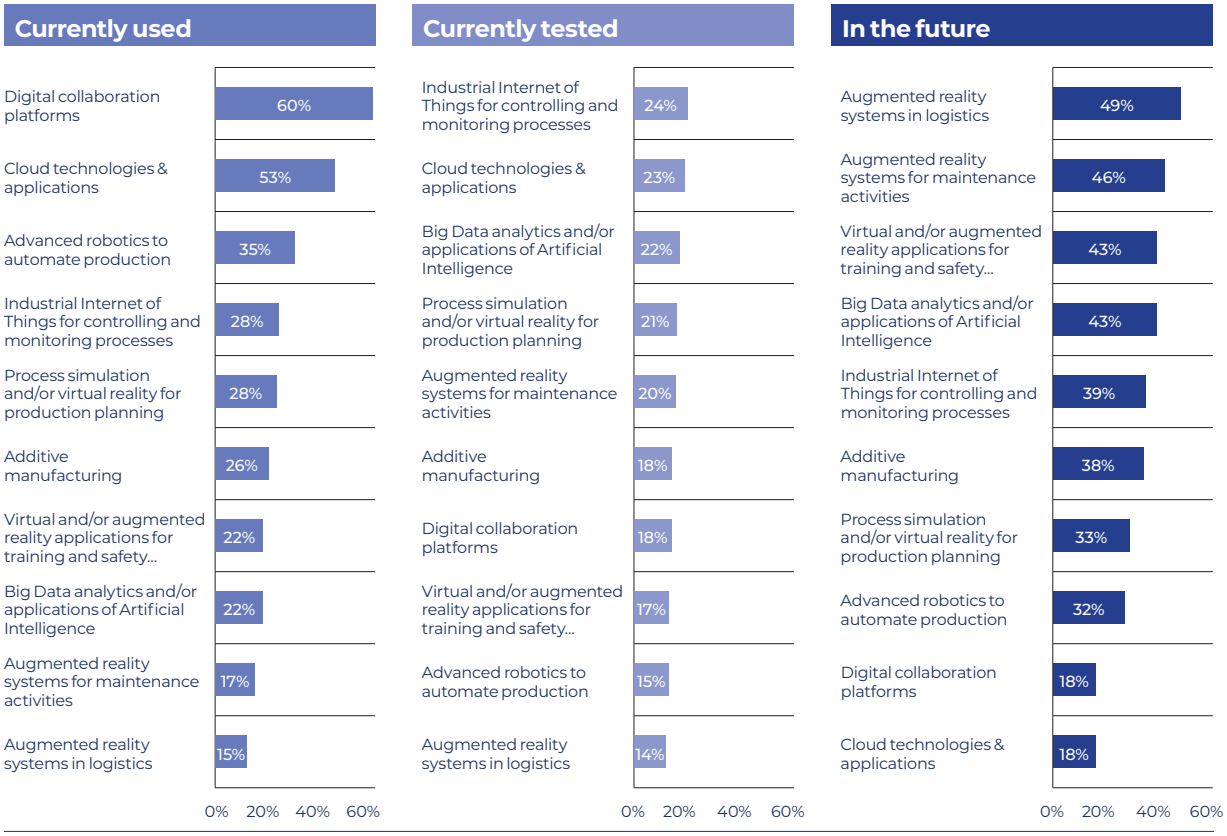
Current chemical engineering university courses are strong on conveying the fundamentals of thermodynamics, chemical kinetics, and transport processes. All have significant digital skills components including competence in the use of simulation tools and control theory and practice. Some have experience of programming and software management. The core Process Systems Engineering capability of optimisation, dynamics, advanced control, and supply chain analysis are covered in some Universities where there is respective expertise. In some cases, this is seen as a postgraduate expertise.[323] There are emerging undergraduate courses and post-graduate training centres in the digital technologies underpinning the development of industry 4.0. The evolving area of data science is, currently, a specialist area in which chemists and chemical engineers are not highly involved. However, there is a rapidly developing skills base in chemistry, physics and material science with respect of informatics, data science, machine learning, robotics and AI.

Future needs- outlook

To make the best use the digital transformation of the chemical sector, it will be increasingly important to enhance the digital skills competence of the existing workforce in the chemical industry as well as new scientists and engineers. Digital skills requirements evolve very fast (see the **Figure below**), making it challenging to keep pace with.

Engineers and scientists will need to develop an appreciation of the strengths and limitations of new digital technologies in areas such as data science, machine learning, robotics and artificial intelligence and the ability to apply systems thinking. This will need to be incorporated in University training to complement systems engineering and modelling skills that are covered in modern programmes already. Graduates of these programmes are not yet 'digital natives' but well-trained in applying and critically reflecting the opportunities and limitations of the techniques. The bigger challenge is to upskill the existing workforce of scientists, engineers, process operators and managers, considering the dynamic and fast-paced evolution of digital technologies and skills requirements. This is a very significant task and requires not only education on new tools and techniques but also a change of mindset to place more trust in digital technologies while at the same time retaining a critical view of its limitations.

Expected evolution of digital technologies/skills implementation, as relevant to the European chemical industry.[324]



Note: The share of respondents indicating "not important" is not included in the figure. It ranges from 4-22%
Source: Prognos AG (2019), based on European wide chemical industry stakeholder survey (2018), n=290-376.

SUSCHEM

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3. Advanced Processes

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Endnotes

Abbreviations

2PP	Two-Photon Polymerization
AI	Artificial Intelligence
AM	Additive manufacturing
APIs	Active pharmaceutical ingredients
AWE	Alkaline water electrolysis
B2B	Business to business
BBI JU	The Bio-based Industries Joint Undertaking
CAD	Computer-aided Design
CAGR	Compound Annual Growth Rate
CAM	Computer-aided Manufacturing
CAPEX	Capital expenditure
CF	Cohesion Fund
CFD	Computational fluid dynamics
CRM	Critical raw materials
CO	Carbon monoxide
CO_2	Carbon dioxide
CO_2-eq	Carbon dioxide equivalent
DES	Deep eutectic solvents
EAFRD	European Agricultural Fund for Rural Development
EIC	European Innovation Council
EMFF	European Maritime and Fisheries Fund
EoL	End of Life
EPDM	Ethylene propylene diene monomer
ERC	European Research Council
ERDF	European Regional Development Fund
ESF	European Social Fund
ESIF	European Structural and Investment Funds
ETP	European Technology Platform
EU	European Union
FRP	Fibre-reinforced Plastic
FT	Fischer-Tropsch
GHG	Greenhouse gas
HEU	Horizon Europe – The proposed European Union Framework Programme for Research and Innovation (2021-2027)
HPC	High performance computing
Horizon 2020	The European Union Framework Programme for Research and Innovation (2014-2020)
HS&E	Health, safety and environment
IB	Industrial biotechnology
ICT	Information and communications technology
IoT	Internet of Things
IPCEI	Important Projects of Common European Interest
ISO	International Organization for Standardization
JRC	Joint Research Centre
LCA	Life-cycle assessment
KETs	Key Enabling Technologies
ML	Machine Learning
MOF	Metal Organic Framework
NIR	Near infrared
NTP	National Technology Platform
OPEX	Operating expenditure
OLED	Organic Light Emitting Diode
PA	Polyamide
PAT	Process Analytical Technologies
PC	Polycarbonate
PE	Polyethylene
PEF	Polyethylene furanoate
PEM	Polymer electrolyte membrane
PET	Polyethylene terephthalate
PLA	Polylactic acid
PP	Polypropylene
PPP	Public-Private-Partnership
PS	Polystyrene
PU	Polyurethane
PV	Photovoltaic
RTOs	Research & Technology Organisations
SOE	Solid oxide electrolysis
SIRA	Strategic Innovation and Research Agenda
SMEs	Small and Medium sized Enterprises
SPIRE cPPP	The Sustainable Process Industry through Resource and Energy Efficiency contractual PPP
TRLs	Technology Readiness Levels
UN SDGs	United Nations Sustainable Development Goals
UV	Ultraviolet

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