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Identification of Priority Topics in the Field of Sustainable Chemistry

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Identification of Priority Topics in the Field of Sustainable Chemistry

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Abstract

To enable the ISC_3 a quick start in its substantive work, the customers (UBA/BMUB) have commissioned the drafting of three studies. The objective of this study was to identify to identify priority topics, i.e. technical solutions, concepts, business models etc., in the field of Sustainable Chemistry. A desktop research has been performed to elucidate specific challenges and recent innovations in different fields of application and industrial sectors: 1) petrochemicals and base chemicals, 2) polymers,3) agrochemicals (pesticides), 4) fertilisers, 5) coatings, dyes, pigments and adhesives, 6) detergents, cleaning agents and personal care products, 7) chemical fibres, 8) construction chemistry , 9) pharmaceuticals, 10) nanomaterials. Other chapters depict funding programmes and awards related to sustainable chemistry in the EU and the U.S., as well as tax instruments, funding and regulatory framework conditions supporting sustainable chemistry in Brazil as an example of a major emerging region with strong chemical industry.

Finally, two separate chapters have been dedicated to the issue of sustainability assessment, in which a more in-depth discussion on the aspect of sustainability is provided for two examples: a) construction materials for thermal insulation as an application field and b) different synthesis routes from fossil and renewable feedstock to acrylic acid.

Kurzbeschreibung

Um dem ISC_3 einen schnellen Einstieg in die fachliche Arbeit zu ermöglichen, haben die Auftraggeber (UBA/BMUB) die Erstellung dreier Studien beauftragt. Ziel dieser Studie war die Identifizierung prioritärer Themen, d.h. technischer Lösungen, Konzepte, Geschäftsmodelle etc. im Bereich der nachhaltigen Chemie. Eine Literaturrecherche wurde durchgeführt, die spezifische Herausforderungen und jüngste Innovationen in verschiedenen Anwendungsfeldern und Sektoren beleuchten: 1) Petro- und Basischemie, 2) Polymere, 3) Agrochemikalien (Pflanzenschutz), 4) Düngemittel, 5) Farbstoffe, Lacke, Pigmente und Klebstoffe, 6) Wasch-, Reinigungs- und Körperpflegemittel, 7) Chemiefasern, 8)Bauchemie, 9) Pharmazeutika und 10) Nanomaterialien. Weitere Kapitel beschreiben Förderprogramme und Auszeichnungen im Bereich der nachhaltigen Chemie in Europa und den USA, sowie Steuerinstrumente, Förder- und regulatorische Rahmenbedingungen am Beispiel Brasilien als Schwellenland. Zum Schluss wurden zwei Kapitel der Thematik der Nachhaltigkeitsbewertung gewidmet, in diesen werden Aspekte der Nachhaltigkeit anhand von zwei Beispielen diskutiert: a) Baumaterialien zur Wärmedämmung als Anwendungsbereich und b) verschiedene Syntheserouten auf Basis fossiler und nachwachsender Rohstoffe zu Acrylsäure.

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API	Active Pharmaceutical Ingredient
CEN	Comité Européen de Normalisation, European Committee for Standardisation
CHP	Combined Heat and Power
EPA	Environmental Protection Agency (U.S.)
EPSP	5-enolpyruvylshikimate-3-phosphate
FP7	7^{th} EU Framework Programme for Research
GHG	Greenhouse Gases
GWP	Global Warming Potential
ISC_3	International Sustainable Chemistry Collaborative Centre
LCA	Life Cycle Assessment
LDPE	Low Density PolyEthylene
LED	Light-Emitting Diode
NGO	Non-Governmental Organisation
ODP	Ozone Depletion Potential
OECD	Organisation for Economic Co-operation and Development
OLED	Organic light-emitting diode
PCM	Phase Change Material
PSC	Parameters for Sustainable Chemistry
PUR	Polyurethane
R&D	Research and Development
SDGs	Sustainable Development Goals
SME	Small/Medium sized Enterprise
UBA	Umweltbundesamt, German Environment Agency
VOC	Volatile Organic Compound
WHO	World Health Organisation

Summary

The study presented here has been devoted to identifying priority topics in the field of sustainable chemistry. It focuses on innovations in some of the important areas of production and application of chemicals thereby trying to identify sustainable chemistry approaches. Having this design of the study in mind, it is clear that numerous approaches cited will not be assessed as "sustainable" in a broader perspective, while others will turn out as incremental developments towards one or more dimensions or indicators of sustainability. The ISC$_3$ project group did not attempt to assess sustainability of the huge amount of process and product innovations in the chemical and pharmaceutical industry, but strived to identify developments that contribute to solve grand societal challenges such as health, food security, secure, clean and efficient energy, secure supply of clean water, climate change etc. The Sustainable Development Goals (SDGs) represent the major comprehensive principle, in which sustainable chemistry is embedded and the definition of Sustainable Chemistry as a concept developed by the German Environment Agency in consultation with national and international stakeholders provides guidance on how to regard sustainable chemistry in a holistic approach. Prioritisation of the numerous research and innovation efforts in the various chemical sectors is difficult, but in any case requires careful assessment of sustainability via LCA studies and other holistic assessment methods to investigate impacts of a new process or product. Novel, highly innovative industry fields or sectors provide the opportunity of introducing sustainable thinking early on and in the whole value chain. The SDGs are important criteria for prioritisation of actions. Further aspects relevant for a prioritisation of activities include the expected effectiveness of measures, technologies and (project and/or R&D) activities in terms of a rapid, efficient and effective implementation of sustainable chemistry and opportunities/possibilities for start-ups and SMEs to participate.

The question has already been raised, which innovations can be included under "sustainable chemistry". With respect to the large number of innovations found from desktop research, this question can only be answered for a more or less representative example. The approach selected here does not target the actual substance itself, as a substance or a product is never sustainable per se, but instead how a substance or (raw) material is used in a particular application. "Thermal building insulation" was chosen as an example because of its enormous importance for energy efficiency and climate protection on one hand and because of the diversity of chemicals and materials used in this field. The innovations show different ecological goals and refer to various stages in the life cycle. This underlines the difficulty in assessing materials in the context of sustainable chemistry.

To assess the sustainability of innovative solutions in the field of thermal insulation, two approaches have been used:

- a set of quantifiable indicators for sustainable chemistry (Parameters for Sustainable Chemistry - PSC) from a study which has been performed for the Umweltbundesamt
- a number of objectives chosen from the Sustainable Development Goals (SDGs) which are directly connected to sustainable chemistry or to objectives which are considerably influenced by the use of chemicals, e.g. health issues, energy efficiency, waste prevention.

The PSC were primarily developed for enterprises which produce chemical substances or use them in the manufacture of materials. Therefore, most indicators are substance-related in conjunction with the respective production process and producer specific situation as well as its success in the market. Therefore, only some of these indicators could be used for the assessment of insulating materials. In these cases, relative estimates were made, because data were not available or not comparable. As to the objectives derived from the SDGs, qualitative assessments and/or relative evaluations (solution A is better than solution B…) were carried out. One may conclude from this example

- that a holistic assessment is lacking of "sustainable chemistry indicators" to be defined and – at best – quantified

- that a number of innovative approaches yield more sustainable solutions than materials or processes used up to now with respect to several objectives derived from the SDGs
- that also in this case, their contribution to other objectives cannot be assessed or could also be negative
- that specific conditions related to the building (e.g. local climate, main construction material) influence the results of the assessment.

A second assessment example investigates different production routes for acrylic acid as the target product, based on different feedstocks, again using the PSC. Generally, the biomass routes are advantageous compared to fossil routes in terms of GHG emissions, but also characterised by a substantially higher energy demand due to lower overall process efficiency. Moreover, other impacts have to be taken into account such as land use and a high water footprint of crop cultivation. Sucrose and starch biomass also have the additional critical aspect of potential food and feed competition. Biomass utilisation efficiency for the production of some precursor molecules such as ethylene or propylene can be very low, i.e. several tons of biomass are required to produce a ton of product. In this sense it is advised not only to perform a cradle to gate LCA for one given route, but to also compare different utilisation routes for a given feedstock to identify the best options. This is particularly recommended for feedstock of limited availability, such as native biomass.

Due to the often highly divergent requirements of various industrial sectors, the search for innovations was focused on specific fields of application, respectively the sectors of the chemical industry.

Petrochemicals and base chemical production is based on well established high volume processes from fossil feedstock, i.e. oil, Naphtha, coal and natural gas. With respect to GHG emissions, a high reduction potential is expected from game changing technologies aiming at novel pathways utilizing alternative (low carbon footprint) feedstock, although the cost-effectiveness of such new technologies is not yet demonstrated. Focus of innovation activities is the use of either biomass or CO_2 as feedstock. For biomass, focus has to be on second generation biomass, e.g. lignocellulosic biomass to avoid food competition. The use of CO_2 as carbon source is emerging, demonstration plants are in operation e.g. for CO_2-based methanol (Carbon Recycling International CRI in Iceland) and for synthetic fuels from CO_2 (sunfire in Germany). These routes require hydrogen, which has to be produced from renewable energy sources to yield a positive process carbon footprint.

The field of **polymers** has to be divided into large commodity polymers, for which the same approaches and prerequisites are valid as for the petrochemicals, and specialty polymers which are highly diverse and dynamic. For the latter, new functionalities are the main target of innovation activities and sustainability has to be assessed. New bio-based polymers include for instance polyamide 11 derived from castor oil or poly-3-hydroxybutyrate (PHB). An important area is recycling of polymers, which requires stronger attention and will need matching value chain collaboration and logistics to be in place.

In the **agrochemicals (pesticides)** industry, only a few innovative approaches could be identified. This is no doubt due to the fact that this is a very strictly regulated area and in that western industrialized nations industry has considerably reduced its research effort due to a concentration on GM seeds. Microencapsulation of the active substance or nanopesticides (active substance is built into a small particle < 100 nanometers) can be regarded as an innovation but currently there are too many questions open, e.g. the risk of further contamination of water and soil due to the improved transport and longer "lifetime" of the active substances. The innovation approaches described in this chapter refer to biochemical pesticides, e.g. microbial pesticides and natural plant and insect regulators.

It is of critical importance to introduce agricultural practices that allow build up of organic matter in the soil to reduce soil erosion and increase soil fertility and soil health. With this in mind, new organic

fertilisers (e.g. a combination of humic acid and mineral fertiliser) can be regarded as innovation. Further approaches focus an resource recovery, e.g. feedstock change by new or more effective processes for the recovery of nutrients (here above all phosphorus) from wastewater/waste, or increasing the efficiency in the use of the nutrient input (e.g. slow release/controlled release), nitrification and urease inhibitors, or the development of optimized application techniques for slower release and better plant uptake. Optimized production techniques include biomethane as a renewable source of hydrogen for the Haber-Bosch-process or the minimisation of precious metal loss and greenhouse gas emissions in the production of nitric acid using the Ostwald process. But one has to keep in mind that these innovations need further input of materials and energy. Therefore an LCA approach is always necessary to clear the ecological advantageousness. In addition, an examination by independent third parties on the sustainability of these examples is not available.

Coatings, dyes, pigments and adhesives comprise a complex field with many interfaces or overlaps with other sectors addressed by this study, e.g. specialty polymers, construction chemicals etc. Environmental regulations are a driving force behind the adoption of new coating technologies. Waterborne and high-solids coatings, powders, UV curables, and two-component systems appear to have good growth prospects. Additives belong to a broad and diffuse category of key components in a coating formulation. The focus on green technology, sustainability, nanotechnology, lower cost and safer products has led to the introduction of newer additives and chemistries, thereby still demanding the same or better performance than their traditional counterparts. While many new products claim sustainability benefits, those are often reduced to one impact category. All sustainability indicators have therefore to be assessed carefully.

Requirements for the functional properties of **detergents, cleaning agents and personal care products** differ with their intended use. High performance, low toxicity and high and full biodegradability of the organic components is a prerequisite in many countries. Resource efficiency, resource recovery and use of renewable sources are further important aspects. With regard to the use of renewable sources (palm oil), potential negative impacts such as loss of biodiversity due to the necessary cultivation areas with monocultures and intensive agricultural use has to be excluded. Therefore, an LCA approach is always necessary to clear the ecological advantageousness. Currently, detailed criteria (ecological, societal and economic, including life cycle assessment) are developed within a new European norm on Bio-surfactants and Bio-solvents (CEN: mandate M/491 for Bio-surfactants and Bio-solvents). LCA for detergents e.g. showed that in addition to the composition, the product design with regard to simple and economical dosage is a major influencing factor for the overall consumption. Innovation approaches include renewable resources, increased application efficiency, improvement of production processes and of the entire life cycle.

The field of **chemical fibres** was screened with focus on technical applications. A broad variety of developments already on the market and innovations was found. Incremental steps towards sustainability could be identified especially in the use of – up to now – waste fibre residues (e.g. as basis for chemicals), in new and better production processes with higher yields and less waste, in the development of applications for nanocellulose and related compounds, in the substitution of steel and other non-renewable compounds by fibres from plants and trees. Fibre re-enforced polymers (FRP) have ever increasing importance for light-weight constructions. On the other hand, most current combinations of fibres with polymers impede the recovery of both compounds after use.

The **construction chemistry** sector is complex and demarcation is difficult. Besides typical chemicals used for building purposes such as adhesives, coatings, paints, wood preservers and fillers, an enormous number of other chemicals are used as additives for the production of cement, bricks and other materials of high volume. Trends in the production and use of materials follow quite different goals such as low energy consumption, decreased emission of greenhouse gases (GHG), less hazardous properties thus contributing incrementally to one or more SDGs. For the production of cement as the most important construction material, lower energy consumption and use of waste fractions are of high importance. As to the products, many innovations were found in the literature, e.g. (infra-) lightweight concrete recipes, thinner insulating material on the market and under development, wood preservation without chemicals, building materials with self-healing properties, enhanced protection of surfaces. Moreover, many attempts focus on the substitution of traditional by renewable raw materials.

The **pharmaceutical** industry is currently undergoing a transition in manufacturing towards the use of the Green Chemistry principles to develop atom-efficient and more benign synthesis strategies for reaction steps widely used for production of active pharmaceutical ingredients. Reduction of the environmental impact of pharmaceutical products is based on a rational design of pharmaceutical compounds to improve for instance degradability. Other important areas which contribute to the SDGs entail novel drugs for treatment of rare diseases, affordable drugs, dedicated drugs for children or improved patient treatment using novel drug delivery systems.

The field of **nanomaterials** enables a large range of applications, from energy storage, air and water purification, surface protection up to catalysis and drug delivery just to mention a few. Most nanomaterials applications aim at superior materials characteristics or improved customer benefits based on enhanced or additional functionalities. The production, use and life-cycle impact of nanomaterials have to be carefully assessed case by case, to identify, which developments and applications are to be flagged as sustainable chemistry. The safety of nanomaterials including potential ecological and health implications of these materials, is subject to many research programmes.

A separate chapter of this study depicts funding programmes and awards related to sustainable chemistry in the EU and the U.S as examples. Many different funding mechanisms exist including bottom-up programmes for fundamental research via funding programmes with specific calls on defined topics or specific awards.

Finally, another chapter summarises tax instruments, funding and regulatory framework conditions supporting sustainable chemistry in Brazil as an example of a major emerging region with strong chemical industry.

Zusammenfassung

Ziel der vorliegenden Studie war die Identifizierung prioritärer Themenfelder im Bereich der nachhaltigen Chemie. Ihr Schwerpunkt liegt auf Innovationen in einigen wesentlichen Bereichen der Produktion und Anwendung von Chemikalien, wobei jeweils Ansätze nachhaltiger Chemie identifiziert werden sollen. Führt man sich dieses Design der Studie vor Augen, dann ist es klar, dass viele der hier zitierten Ansätze nicht als „nachhaltig“ in einer umfassenden Sichtweise bewertet werden können, andere sich als inkrementelle Entwicklungen im Sinne einer oder mehrerer Dimensionen oder Indikatoren der Nachhaltigkeit herausstellen. Die ISC$_3$-Projektgruppe verzichtete darauf, die Nachhaltigkeit der enormen Zahl an Prozess- und Produktinnovationen in der chemischen und pharmazeutischen Industrie zu prüfen, sondern konzentrierte sich darauf, Entwicklungen zu identifizieren, die dazu beitragen, großen gesellschaftlichen Herausforderungen wie Gesundheit, Nahrungsmittelversorgung, sichere und effiziente Versorgung mit Energie, sichere Versorgung mit sauberem Wasser, Klimaschutz usw. zu begegnen. Das wesentliche übergreifende Leitbild ist durch die „Sustainable Development Goals“ (SDG‘s) der Vereinten Nationen vorgegeben, wobei nachhaltige Chemie sich darin einfügt; das Konzept Nachhaltiger Chemie, wie es vom Umweltbundesamt in Zusammenarbeit mitnationalen und internationalen Akteuren entwickelt wurde, ermöglicht es, nachhaltige Chemie in einem ganzheitlichen Ansatz zu betrachten. Es ist schwierig, die zahlreichen Anstrengungen bei Forschung- und Innovationen in unterschiedlichen Bereichen der Chemie zu priorisieren, da hierzu sorgfältige Abschätzungen der Nachhaltigkeit mit Hilfe von LCA und anderen ganzheitlich orientierten Bewertungsansätzen zur Untersuchung der Folgen

neuer Reaktionen bzw. Produkte erforderlich sind. Die SDG's stellen wichtige Kriterien für die Prioritätensetzung dar. Weitere Aspekte, die für die Priorisierung von Aktivitäten von Bedeutung sind, beinhalten die Effektivität von Maßnahmen, Technologien und sonstigen (Projekt- oder FuE-) Maßnahmen mit Bezug auf eine schnelle, effektive wie effiziente Umsetzung nachhaltiger Chemie sowie der Chancen und Möglichkeiten, die sich für start-ups und KMU ergeben.

Wie bereits erwähnt, stellt sich die Frage, welche Innovationen zur "nachhaltigen Chemie" gezählt werden können. Angesichts der großen Zahl innovativer Ansätze, die bei der Desktop-Recherche gefunden wurden, lässt sich diese Frage nur an mehr oder weniger repräsentativen Beispielen beantworten. Der hier gewählte Ansatz zielt nicht auf die jeweils betrachtete Substanz, da eine Chemikalie oder ein Produkt per se nicht nachhaltig sein können, sondern auf das Verhalten einer Substanz oder eines (Roh-) Materials bei einer bestimmten Anwendung. Als Beispiel wurde die thermische Gebäudedämmung ausgewählt, weil diese Anwendung einerseits eine enorme Bedeutung für Energieeffizienz und Klimaschutz hat, und dafür andererseits eine Vielzahl unterschiedlicher Chemikalien und Materialien gebraucht wird. Die betrachteten Innovationen fokussieren auf unterschiedliche ökologische Ziele und beziehen sich auf verschiedene Phasen des Produktlebens. Dies unterstreicht die Schwierigkeiten bei der Einschätzung von Materialien im Kontext nachhaltiger Chemie.

Um die Nachhaltigkeit innovativer Lösungen im Bereich thermische Gebäudeisolation abzuschätzen, wurden zwei Ansätze verwendet:

- Eine Reihe quantifizierbarer Indikatoren für nachhaltige Chemie (Parameters for Sustainable Chemistry - PSC) aus einer im Auftrag des Umweltbundesamts erstellten Studie,
- Eine Anzahl von aus den SDG's ausgewählten Zielen, die entweder in direktem Zusammenhang mit nachhaltiger Chemie stehen oder durch die Anwendung von Chemikalien erheblich beeinflusst werden, wie etwa Schutz der Gesundheit, Energieeffizienz, Abfallvermeidung.

Die PSC wurden primär für Unternehmen entwickelt, die Chemikalien herstellen oder bei der Herstellung von Materialien einsetzen. Daher konnten nur einige dieser Indikatoren für die Bewertung von Isoliermaterialien eingesetzt werden. Dabei erfolgte eine Beschränkung auf relative Abschätzungen zwischen einzelnen Materialien, wenn Daten nicht vorhanden oder vergleichbar waren. Bei den aus den SDG's abgeleiteten Zielen wurden qualitative Abschätzungen und/oder relative Bewertungen (Lösung A ist besser als Lösung B…) vorgenommen. Aus diesem Beispiel lässt sich schlussfolgern,

- dass für eine ganzheitliche Bewertung noch Indikatoren für nachhaltige Chemie fehlen, die zu definieren und – vorzugsweise – quantifizieren sind,
- dass eine Anzahl innovativer Ansätze mit Blick auf eine Reihe von Zielen aus den SDG's zu nachhaltigeren Lösungen führen als bisher genutzte Materialien oder Verfahren,
- dass auch in solchen Fällen Beiträge zu anderen Zielen nicht abschätzbar sind oder auch kontraproduktiv sein können,
- dass spezifische Rahmenbedingungen für das jeweilige Gebäude (z.B. lokale Klimabedingungen, wesentliche Konstruktionsmaterialien) die Ergebnisse der Abschätzung beeinflussen.

Ein zweites Bewertungsbeispiel bezieht sich auf verschiedene Möglichkeiten der Herstellung von Acrylsäure ausgehend von unterschiedlichen Rohstoffen wiederum unter Verwendung der PSC. Generell sind die auf Biomasse basierenden Reaktionswege im Vergleich zu fossilen günstiger im Hinblick auf THG-Emissionen, allerdings weisen sie einen höheren Energiebedarf auf Grund niedrigerer Effizienz des gesamten Reaktionswegs auf. Außerdem müssen weitere Folgen wie höherer Flächenbedarf und ein hoher Wasser-Fußabdruck für den Anbau berücksichtigt werden. Bei Biomasse aus Saccharose und Stärke sollte auch der kritische Aspekt potenzieller Konkurrenz zu Nahrungs- und Futtermitteln beachtet werden. Die Effizienz beim Einsatz von Biomasse für die Herstellung von Vorprodukten wie Ethen oder Propen kann sehr gering sein, z.B. sind mehrere Tonnen Biomasse zur Herstellung von einer Tonne Produkt erforderlich. Dieses Problem sollte vor allem bei Rohstoffen mit begrenzter Verfügbarkeit wie nativer Biomasse beachtet werden.

Angesichts der meist sehr unterschiedlichen Anforderungen verschiedener Industriesektoren konzentrierte sich die Suche nach Innovationen auf spezifische Anwendungsbereiche bzw. Sektoren der Chemieindustrie.

Zur **Herstellung von Petro- und Basischemikalien** greift man auf lange bekannte Prozesse mit hohen Reaktionsvolumina zurück, die von fossilen Rohstoffen wie Öl, Naphtha, Kohl oder Erdgas ausgehen. Wegweisende Technologien, die auf neuen Reaktionswegen unter Nutzung alternativer Rohstoffe (mit geringem Carbon Footprint) beruhen, weisen ein hohes Reduktionspotential für THG auf; allerdings ist das Kosten-Effektivitäts-Verhältnis solcher neuer Technologien noch nicht geklärt. Im Fokus der Innovationen steht die Nutzung von Biomasse oder CO_2 als Rohstoff. Bei Biomasse liegt der Schwerpunkt bei Rohstoffen der zweiten Generation, z.B. Lignocellulose, zur Vermeidung einer Konkurrenz mit Nahrungsmitteln. Die Nutzung von CO_2 als Kohlenstoffquelle nimmt zu; Demonstrationsanlagen z.B. für CO_2-basiertes Methanol (Carbon Recycling International CRI in Island) und für synthetische Treibstoffe aus CO_2 (Sunfire in Deutschland) laufen. Für diese Prozesse benötigt man Wasserstoff, der aus erneuerbaren Energien gewonnen werden muss, um einen geringen Carbon Footprint für den Prozess zu erzielen.

Im Bereich **Polymere** muss zwischen den Massenkunststoffen, für die die gleichen Ansätze und Voraussetzungen wie für die Petrochemie gelten, und Spezialitäten unterschieden werden, die sehr unterschiedliche Strukturen aufweisen und sich dynamisch entwickeln.

Im Bereich der **Agrochemikalien (Pestizide)** wurden nur wenige innovative Ansätze identifiziert. Dies hängt zweifellos damit zusammen, dass es sich um einen stark regulierten Sektor handelt, und die Chemieindustrie in den westlichen Industrienationen ihre Forschungsaktivitäten auf genmanipulierte Organismen konzentriert hat. Der Einschluss der Wirkstoffe in Mikrokapseln oder Nanopestizide (bei denen der Wirkstoff in Teilchen < 100 nm eingebaut wird) können als Innovationen angesehen werden; allerdings sind zur Zeit noch viele Fragen unbeantwortet, wie etwa das Risiko der Kontamination von Wasser und Boden infolge des verbesserten Wirkstoff-Transports und einer längeren „Lebensdauer" der Wirkstoffe. Die in diesem Abschnitt beschriebenen Innovationen beziehen sich auf biochemische Pestizide, z.B. mikrobiologisch wirksame Substanzen und Naturstoffe mit herbizider oder insektizider Wirkung.

Die Einführung landwirtschaftlicher Methoden zum Aufbau organischer Substanz im Boden zur Reduzierung von Erosion und zur Verbesserung von Bodenfruchtbarkeit und Bodengesundheit ist von höchster Bedeutung. Daher können neue **organische Düngemittel** (eine Kombination von Huminsäuren und Mineraldünger) als Innovation angesprochen werden. Weitere Bemühungen konzentrieren sich auf die Wiedergewinnung von Ressourcen aus Abwasser oder Wasser, so z.B. durch neue oder effektivere Prozesse für das Nährstoffrecycling (vor allem Phosphor), bzw. eine Steigerung der Effizienz bei der Nährstoffausbringung (z.B. langsame oder kontrollierte Freisetzung), Nitrifikation und Urease-Inhibitoren, oder die Entwicklung optimierter Anwendungstechniken für eine langsamere Abgabe und bessere Aufnahme durch Pflanzen. Optimierte Produktionsprozesse in diesem Bereich umfassen die Nutzung von Biomethan als erneuerbare Quelle für Wasserstoff im Haber-Bosch-Verfahren oder die Minimierung des Verlustes wertvoller Metalle sowie von THG-Emissionen bei der Herstellung von Salpetersäure mit dem Ostwald-Verfahren. Allerdings ist dabei zu beachten, dass diese Innovationen einen zusätzlichen Material- und Energieaufwand bedeuten. Daher ist stets eine LCA zur Abklärung der ökologischen Vorteile erforderlich. Zusätzliche Prüfungen der Nachhaltigkeit dieser Beispiele durch unabhängige Dritte sind nicht verfügbar.

Beschichtungen, Farben, Pigmente und Klebstoffe stellen einen komplexen Bereich mit zahlreichen Schnittstellen oder Schnittmengen mit anderen Bereichen dieser Studie dar, z.B. mit Spezialpolymeren, Bauchemikalien usw. Die Umweltgesetzgebung wirkt als Treiber für die Entwicklung neuer Beschichtungstechnologien. Beschichtungen auf wässriger Basis sowie solche mit hohem Feststoffanteil, Pulver, UV-härtbare und Zwei-Komponenten-Systeme scheinen gute Wachstumsperspektiven zu haben. In Formulierungen für Oberflächenbeschichtung stellen Additive eine große und breit gestreute Gruppe von Schlüsselkomponenten dar. Der Fokus auf grüne Technologien, Nachhaltigkeit, Nanotechnik, niedrigere Kosten und sicherer Produkte führte zur Einführung von neueren Additive und stofflichen Systemen, wobei gleiche oder höhere Leistung im Vergleich zu den eingeführten Wettbewerbsprodukten erwartet wird.

Anforderungen an die funktionalen Eigenschaften von **Detergentien, Reinigungsmittel und Körperpflegemittel** differieren mit der jeweiligen Anwendung. Hohe Wirksamkeit, geringe Toxizität, sowie rasche und völlige Bioabbaubarkeit der organischen Bestandteile sind in vielen Ländern prinzipielle Bedingungen. Ressourceneffizienz, Verwertung der Ressourcen und die Nutzung nachwachsender Rohstoffe stellen weitere wichtige Aspekte dar. Im Hinblick auf die Nutzung erneuerbarer Stoffe (Palmöl) müssen potenzielle negative Auswirkungen wie Verlust an Biodiversität auf Grund der notwendigen Anbaufläche mit Monokulturen und intensiver Landwirtschaft ausgeschlossen werden. Daher ist eine LCA-Betrachtung zur Abschätzung der ökologischen Vorteilshaftigkeit immer erforderlich. Zur Zeit werden im Rahmen einer neuen europäischen Norm detaillierte Kriterien (ökologisch, sozial und ökonomisch, einschließlich LCA) zu Bio-Tensiden und Bio-Lösemitteln (CEN: mandate M/491 for Biosurfactants and Bio-solvents) entwickelt. So zeigten LCA‘s für Detergentien, dass zusätzlich zu der Zusammensetzung des Produkts dessen Design hinsichtlich einfacher und sparsamer Dosierung ein wesentlicher Faktor für den Gesamtverbrauch darstellt. Innovative Ansätze beinhalten die Nutzung erneuerbarer Rohstoffe, höhere Effizienz bei der Anwendung, Verbesserung von Produktionsprozessen und des gesamten Lebenszyklus.

Beim Bereich **Chemiefasern** lag der Fokus der Studie auf technischen Anwendungen. Dabei fand sich eine breite Vielfalt von Entwicklungen, sowohl Produkte im Markt als auch Innovationen. Inkrementelle Schritte in Richtung Nachhaltigkeit ließen sich speziell bei bisher entsorgten Faserresten (z.B. als Rohstoff für Chemikalien), bei neuen und besseren Produktionsprozessen mit höheren Ausbeuten und weniger Abfall, bei der Entwicklung von Anwendungen für Nanozellulose und verwandte Verbindungen, bei der Substitution von Stahl und anderer nicht-erneuerbarer Stoffe durch Pflanzen- und Holzfasern feststellen. Faserverstärkte Polymere (FRP) haben eine steigende Bedeutung für Leichtgewichts-Konstruktionen. Andererseits behindert die aktuelle Kombination von Fasern mit Polymeren die Verwertung beider Komponenten nach Gebrauch.

Der Bereich der **Bauchemie** ist komplex, seine Abgrenzung schwierig. Neben typischen Chemikalien für das Bauwesen wie Klebstoffe, Beschichtungsmitteln, Farben, Holzschutzmitteln, Spachtelmassen findet eine enorme Menge anderer Chemikalien als Additive bei der Herstellung von Zement, Ziegeln und anderen Materialien mit hohem Produktionsvolumen Anwendung. Trends bei Herstellung und Verwendung von Materialien hängen mit unterschiedlichen Zielen zusammen wie verringertem Energieaufwand, abnehmender Emission von THG, weniger gefährlichen Eigenschaften, so dass sie inkrementell zu einem oder mehreren SDG’s beitragen. Bei der Zementherstellung als wichtigstem Baumaterial stehen ein geringerer Energieverbrauch und die stoffliche Nutzung von Abfallfraktionen im Fokus. Auf Seite der Produkte lassen sich zahlreiche Innovationen wie z.B. Rezepturen für (Infra-) Leichtgewichtsbeton, dünnere Werkstoffe für die Isolierung auf dem Markt wie auch in der Entwicklung, Holzschutz ohne Chemikalien, Baumaterialien mit selbstheilenden Eigenschaften, verbesserter Schutz von Oberflächen. Ferner konzentrieren sich viele Ansätze auf die Substitution konventioneller durch erneuerbare Rohstoffe.

Die **Pharmazeutische Industrie** macht gerade eine Transformation in Richtung auf die Anwendung von Green Chemistry-Prinzipien durch, wobei atom-effiziente und mildere Synthese-Strategien für Reaktionsschritte, die bei der Herstellung pharmakologisch wirksamer Stoffe große Bedeutung haben, in der Entwicklung sind. Die Verringerung der Umweltauswirkungen von Pharmaka fußt auf einem gezielten Design der Wirkstoffe, z.B. zur Verbesserung der Abbaubarkeit. Andere wichtige Entwicklungen, die zu den SDG’s beitragen, beinhalten neue Wirkstoffe zur Behandlung seltener Krankheiten, erschwingliche Arzneimittel, spezielle Medikamente für Kinder oder verbesserte Behandlung von Patienten mit fortgeschrittenen Systemen zur Wirkstoffapplikation.

Das Feld der **Nanomaterialien** macht eine große Zahl von Anwendungen zugänglich, angefangen von der Energiespeicherung, Luft- und Wasserreinhaltung, Schutz von Oberflächen bis zu Katalyse und Wirkstoffapplikation, um nur einige zu nennen. Die meisten Anwendungsfälle von Nanomaterialien zielen auf überlegene Eigenschaften der Materialien oder erhöhten Nutzen für den Anwender auf Grund verbesserter oder zusätzlicher Funktionalitäten, Herstellung, Nutzung und Auswirkungen des Lebenszyklus von Nanomaterialien müssen sorgfältig fallweise bewertet werden, um festzustellen, welche Entwicklungen und Anwendungen unter nachhaltiger Chemie subsummiert werden können. Die Sicherheit von Nanomaterialien einschließlich potentieller Auswirkungen auf Umwelt und Gesundheit ist Gegenstand zahlreicher Forschungsprogramme.

Ein eigener Abschnitt dieser Studie beschreibt Förderprogramme und Auszeichnungen für nachhaltige Chemie am Beispiel der EU und der USA. Es gibt zahlreiche verschiedene Förderprogramme von der Grundlagenforschung bis zu Förderprogrammen zu spezifischen Ausschreibungen für definierte Ziele oder spezielle Branchenpreise.

Abschließend werden in einem weiteren Kapitel steuerliche Instrumente, Förderrahmen und Regelungen, die zur Unterstützung nachhaltiger Chemie dienen könnten, beschrieben. Als Beispiel dient Brasilien als ein großes sich rasch entwickelndes Land mit starker Chemieindustrie

1 Introduction

1.1 Scope of this study

The study “Identification of Priority Topics in the Field of Sustainable Chemistry“ presented here is part of the project “Bundling of Expertise in the area of Sustainable Chemistry” aiming at the preparation and implementation of an International Sustainable Chemistry Collaborative Centre (ISC_3). The project was launched by the German Environment Agency in close cooperation with the German Federal Ministry for the Environment (Environment Research Plan, Project ID 3715 65 499 0). The consortium partners of the project, N^3 Nachhaltigkeitsberatung Dr. Friege & Partner, DECHEMA Gesellschaft für Chemische Technik und Biotechnologie e.V. and BZL Kommunikation und Projektsteuerung GmbH, have been involved in the preparation of this study.

The study has been devoted to identifying priority topics in the field of sustainable chemistry with the focus on recent innovations as well as priority research and development themes, which are needed in particular for a broad industrial implementation of the concept of Sustainable Chemistry. At the recommendation of the ISC3 Advisory Council, that has accompanied the study, the main part of this document has been structured according to different fields of application and/or industrial sectors in order to address the often highly divergent requirements of various industrial sectors. Wherever possible, existing business models for sustainable chemistry, in which industrial players following the chemical sector in the value chain, have been highlighted and case studies have been described. This part of the document represents a comprehensive summary of the study results. For each sector a separate report has been compiled which will be made available to the ISC_3 as basis for their future work.

Following the sector-specific priority topics the study comprises a chapter on funding programs related to sustainable chemistry. The structure and organisation of funding mechanisms is different in each country. For this study the EU and the U.S. have been selected as examples, as both regions have large funding programmes on chemistry which specifically address sustainable chemistry or green chemistry. No attempt has been made to provide comprehensive global overview on funding programs. As part of the original study scope, the ISC3 project team also aimed at the description of existing framework conditions and suitable instruments in different world regions supporting sustainable chemistry. These could include e.g. regulatory measures and governmental incentives. Obviously, the existing landscape is highly complex and differs from country to country. Moreover, most regulatory, tax and other instruments beyond sound management of chemicals and waste[1] (which is subject to a separate study and therefore excluded here) are not specifically dedicated to sustainable chemistry but rather comprise general industry or chemistry policies, which are of limited relevance for the work of the ISC_3. Therefore, this core study presents the situation in Brazil as an example of the policy framework of a major emerging region with strong chemical industry.

Finally, two separate chapters have been dedicated to the issue of sustainability assessment, and a more in-depth discussion on the aspect of sustainability is provided for two examples: a) construction materials for thermal insulation as an application field and b) acrylic acid production, comparing different synthesis routes from fossil and renewable feedstock.

[1] Sound Management of Chemicals is a specific mode of managing chemicals, where specific regulations are applied on the processes of producing, handling, storage, and transport of chemicals. In several publications, also the management of hazardous waste, even if not directly related to chemicals production, is included in this definition, and then the term Sound Management of Chemicals and Waste is used.

1.2 Sustainable Chemistry and the Sustainable Development Goals (SDGs)

Prioritizing innovations in the field of chemistry and pharmaceuticals with respect to sustainability is a complex task. Reliable life cycle assessments proving increased sustainability of new products or emerging technologies in comparison to existing references are at best partly available. The ISC$_3$ project group therefore does not attempt to assess sustainability of the huge amount of process and product innovations in the chemical and pharmaceutical industry, but strives to identify developments that contribute to solve grand societal challenges such as health, food security, secure, clean and efficient energy, secure supply of clean water, climate change etc. In a separate research project commissioned by the German Environmental Agency [2] a set of 25 quantifiable indicators for sustainable chemistry grouped under six core criteria has been developed. A separate chapter of the study provides a more in-depth discussion of sustainability and even contradicting indicators by illustrating the application field of **thermal insulation of buildings** as an example.

Regarding the question of what sustainable chemistry entails, one has to start with the set of 17 Sustainable Development Goals (SDGs) with the 169 subsequent targets. The SDGs represent the major overarching principle, in which sustainable chemistry is embedded. Chemical products or improvements in chemical processes which are in accordance with the ideas behind the SDGs or promote particular goals are considered as part of sustainable chemistry. Chemistry as a materials and solution provider for a large variety of downstream sectors and applications has a large potential impact on the energy and resource efficiency, lifetime, functionality, recyclability, and safety of products in virtually all industrial and consumer areas being more environmentally friendly than alternatives already on the market. Table 1 provides an overview of direct contributions of the chemical industry to the SDGs.

Table 1: Contributions of the chemical industry to selected SDGs

SDG	Contribution of the chemical industry
SDG 2: End hunger, achieve food security and improved nutrition and promote sustainable agriculture	• Biological or biobased agrochemicals (pest control) • New organic fertilizers • New processes for the recovery of nutrients from wastewater/waste • Differentiated use of nutrient input or the development of optimized types of application in agriculture • Approaches for more efficient synthesis of ammonia • Food ingredients
SDG 3: Ensure healthy lives and promote well-being for all at all ages	• Novel drugs to treat rare or “orphan” diseases • New drugs for better quality of care, greater access to medication, more consumer choice, and a competitive marketplace that enhances affordability and public health • Rational design of pharmaceutical compounds by Life Cycle Engineering and biodegradability of pharmaceuticals to reduce environmental imppact • Drug delivery systems for controlled, slow or targeted release or overcoming biological barriers • Implantation materials including materials for additive manufacturing • Coatings against diseases (e.g. insect repellent coatings)

[2] Forschungsprojekt „Beiträge zur Nachhaltigkeitsstrategie: Minderung des Ressourcenverbrauchs in der Chemiebranche durch Instrumente der nachhaltigen Chemie“, FKZ 3713 93 425

SDG	Contribution of the chemical industry
	• Reduction of hazardous chemicals and air, water, and soil pollution and contamination through safe and more benign production processes and products
SDG 6: Ensure availability and sustainable management of water and sanitation for all	• New design of processes requiring less water, new sustainable cooling systems without water, and internal recycling and reuse (Zero Liquid Discharge) • Reduction of the use of fresh water and drinking water resources (sustainable use of alternative sources such as desalination and waste water from urban areas) • Waste water treatment and management • Biodegradable pharmaceuticals and chemical micropollutants to avoid persistent residues in the water system
SDG 7: Ensure access to affordable, reliable, sustainable and modern energy for all	• Advanced materials for renewable energy (photovoltaics, wind turbines, batteries, supercapacitors, thermal energy storage etc.) • Chemical energy storage (e.g. Power-to-X) • Energy efficiency in chemical processing • Materials for energy efficiency of buildings (high performance insulation, reflective coatings, phase change materials, LEDs, OLED etc.) Note: Recyclability, reparability and long-life-time solutions should be envisioned in all these materials and products.
SDG 11: Make cities and human settlements inclusive, safe, resilient and sustainable	• Clean mobility and transport; e.g. materials for batteries, low-carbon fuels etc. • Energy efficient buildings • Coatings for reducing VOCs (inside buildings) and smog/pollutants (building facades)
SDG 12: Ensure sustainable consumption and production patterns	• Resource and energy efficient chemical production • Integration of renewable energy in chemical/pharmaceutical production • Safe production and avoidance of hazardous reagents, solvents and intermediates • Feedstock change to lower carbon footprint feedstock (2nd generation biomass, CO_2 as carbon feedstock for chemicals and fuels) • Closing material cycles as good as possible, waste recovery and valorisation, design for recycle or higher biodegradability • High functional products for downstream applications • Industrial symbiosis with other sectors, to aim at integrated materials/energy flows and resource management
SDG 13: Take urgent action to combat climate change and its impacts	• Chemical processes with lower carbon footprint (process intensification, combined heat and power) • Products for energy savings in downstream sectors and applications (construction, buildings, mobility, lighting, materials lifetime, energy recovery etc.) • "Decarbonisation" of the chemical industry through alternative feedstock, integration of renewables for energy supply

SDG	Contribution of the chemical industry
Goal 14: Conserve and sustainably use the oceans, seas and marine resources for sustainable development	• Biodegradable polymers to reduce marine contamination (micro plastics) • Benign antifouling coatings for marine vessels • foams for oil spillage recovery
SDG 15: Protect, restore and promote sustainable use of terrestrial ecosystems, sustainably manage forests, combat desertification, and halt and reverse land degradation and halt biodiversity loss	• Super absorbent polymers in agriculture for arid and semiarid regions

Source: own compilation

In 2015 the German Environment Agency had launched a consultation with national and international stakeholders in order to comment on a draft description of what sustainable chemistry might be about. This process lead to the description of a Concept of Sustainable Chemistry as submitted to the journal "Sustainable Chemistry and Pharmacy" in the beginning of June 2016. The concept points out objectives and guiding principles of sustainable chemistry and indicates how these can be achieved and realized:

Sustainable chemistry in 100 words

Sustainable chemistry contributes to a positive, long-term development in society, environment and economy. With new approaches and technologies it develops value-creating products and services for the civil society needs.

Sustainable chemistry increasingly uses substances, materials and processes with the least possible adverse effects. Moreover, substitutes, alternative processes and recycling concepts are used, and natural resources are conserved. Thus, damage and impairments to human beings, ecosystems and resources are avoided.

Sustainable chemistry is based on a holistic approach, setting measurable objectives for a continuous process of change. Scientific research and education for sustainable development in schools and vocational training serve as an important basis for this development.

The UBA concept of Sustainable Chemistry evolves the OECD definition of Sustainable Chemistry to a more holistic approach.

OECD: "Sustainable chemistry is a scientific concept that seeks to improve the efficiency with which natural resources are used to meet human needs for chemical products and services. Sustainable chemistry encompasses the design, manufacture and use of efficient, effective, safe and more environmentally benign chemical products and processes. Sustainable chemistry is also a process that stimulates innovation across all sectors to design and discover new chemicals, production processes, and product stewardship practices that will provide increased performance and increased value while meeting the goals, especially achieving welfare and justice for all as well as protecting and enhancing human health and the environment."[3]

The OECD definition has a strong focus on resources and efficiency. Aspects of substance and materials' flow management and new (service oriented) business models are of course also included in the scope of sustainable chemistry.

[3] http://www.oecd.org/env/ehs/risk-management/sustainablechemistry.htm

It has to be pointed out though, that chemical innovations can cause trade-offs or contradicting impacts for different sustainability indicators. The development of guidance to support decision making towards sustainable solutions will be an important remit of the ISC_3 The following examples, which are also highlighted in the subsequent chapters, illustrate the aspect of contradicting impacts:

- Use of 1st generation bio-based feedstock with low CO_2 footprint, e.g. fermentation of sugar, starches, melasses to produce organic acids, amino acids and antibiotics. For these “food/feed” grade feedstock are required to guarantee the quality/suitability of the finished products. Generally, potential competition with food supply has to be evaluated and alternative routes using 2nd generation feedstock should be developed, in this context, also other follow up problems have to be considered, such as land use change and the export of nutrients and materials that are necessary for fertile soils;
- Use of biomass or CO_2 as feedstock results in lower carbon footprint, but causes higher process energy demand (which makes the use of renewable energy sources mandatory, and intrinsically involves the need for more/new materials for energy supply);
- Composite materials provide higher functionalities such as lower weight or higher strength saving energy and raw materials, but causing more difficult end of life treatment or recyclability;
- Thin layers or coatings (e.g. precious metals) reduce materials consumption, but also cause material dissipation (lower recycling rates or more difficult recyclability).

These examples again emphasize the need of LCA studies to investigate sustainability impacts of a new process or product. For many base chemical products (e.g. bulk chemicals, commodity polymers) it can be relatively complex and difficult to expand the LCA beyond a cradle to gate perspective, as the use phase of these products is highly diversified. Also, follow-up implications and rebound effects have to be taken into account in proper evaluations.

1.3 Priority areas for sustainable chemistry

Important areas of innovations for different chemical sectors are summarized in the subsequent chapters. A further prioritisation of the listed activities is challenging. A few thoughts on this are provided subsequently.

1.3.1 Priorities based on sustainability

First of all, it has to be verified case by case, if the provided examples are real approaches towards sustainable chemistry or qualify as more sustainable solutions. On a superficial level, provided examples seem to show benefits in one or more dimensions of sustainable development, e.g. more efficient use of input materials, less waste, smaller carbon footprint as compared to conventional solutions., but verification is required. An in-depth analysis for each innovation remains to be done, but is beyond the scope of this study. For the communication work of ISC_3 it is obviously essential to only highlight case studies as lighthouse examples, if solid sustainability assessment data is available for the given case.

1.3.2 Emerging fields as priority areas

Many areas listed in the following chapters concern traditional chemical sectors and well established production processes and product groups and address the need for a transformation towards e.g. more benign processes, more energy and resource efficient products or the use of non-fossil feedstock. For most of the large volume chemicals, these transition processes are slow and hampered by the need of significant investments and added operational costs vs. already existing production (over)capacities and optimised state of the art process technologies.

In this respect, novel, highly innovative industry fields or sectors provide the opportunity of introducing sustainable thinking early on and to introduce sustainable chemistry in the whole value chain to avoid unsustainable decisions of downstream manufacturers. In addition, such emerging fields usually draw strong attention on public and specialist community levels and the ISC_3 could take an important stakeholder role there. Table 2 illustrates some aspects on the sustainability of graphene and ionic liquids as examples. Other, rapidly growing areas that would also benefit from sustainable chemistry thinking could be named as well. An example is additive manufacturing (3D printing), for which the current innovation and R&D focus is on the manufacturing process, but other aspects such as recycling of components has not yet been addressed appropriately.

Table 2: Examples for highly-innovative industry fields including challenges and innovation needs

Area	Applications (examples)	Challenges	Innovation examples/needs
Graphene	• graphene-based flexible displays, updateable, reusable electronic paper; reduction of paper use and waste • new polymeric graphene batteries with long lifetime, high energy density and short charging cycles • graphene paints with strong corrosion or erosion/weather resistance • weather resistant solar panels with graphene instead of indium tin oxide (ITO)	• Syntheses of highly pure, defect-free graphene by chemical vapor deposition: Copper foil, about 50 µm thick, is the usual material of choice for growing graphene. Once the graphene is grown the copper layer is typically chemically dissolved and destroyed; for every gram of graphene produced more than 2 kg of copper is dissolved • Production of flakes of graphene-like sheets by sequential oxidation and reduction of graphite: the majority of the chemicals involved in the reduction and functionalisation are highly toxic and hazardous, incl. reducing agents such as hydrazine, sodium hydride, and hydrohalic acid and chemical stabilizers, such as porphyrins and pyrenebutyric acid	DTU and partners[4] have developed an electrochemical process reducing the amount of copper to nearly zero: oxygen is dissolved in non-toxic salt water or some other simple electrolyte in between the copper and graphene layer; by applying a reducing potential, the oxidised copper surface is changed back to copper without dissolving it, and at the same time releasing the graphene. Alternative reducing agents have been intensively researched and proposed[5] such as metals, alkaline solutions (e.g., sodium hydroxide and potassium hydroxide), phenols ,alcohols, sugars (e.g., glucose, fructose, sucrose, and natural cellulose), microbes (e.g., Escherichia coli and baker's yeast), and other substances (e.g. glycine, vitamin C, sodium citrate, and protein bovine serumalbumin); limitations are poor reducing abilities and remaining impurities in the final product; a

[4] http://www.nanotech.dtu.dk/english/Samples-newsletter/Apr-15/Graphene

[5] Green preparation of reduced graphene oxide for sensing and energy storage applications, Zheng Bo et al., Scientific Reports 2014, No 4, http://dx.doi.org/10.1038/srep04684

Area	Applications (examples)	Challenges	Innovation examples/needs
			good sustainable alternative is still missing.
Ionic liquids	• solvent in chemical reactions and separation processes • agent for metal deposition processes • hydraulic fluid and lubricant • biomass pre-treatment • dissolving and processing of cellulose • antistatic polymer additive • electrolyte in electronic devices, batteries etc.	• Ionic liquids (ILs) represent a highly diverse group of chemicals, therefore providing a variety of synthesis challenges as well as characteristics, including e.g. toxicity and biodegradability • ILs have often been referred to as green solvents but are not intrinsically green; preparation and purification of the salts often requires large volumes of harmful organic solvents and is accompanied by substantial waste production	Toxicological and ecotoxicological data has been collected for many ILs and the “Thinking in terms of Structure-Activity relationships” (T-SAR) concept has been used to identify the impact of structural elements on (eco)toxicity in various cellular, aquatic and terrestrial test systems Only limited data is available for biodegradability of ILs; there is a strong need for further research ionic liquids from renewable feedstock: e.g. tertiary amine-based ionic liquids from aromatic aldehydes in lignin and hemicellulose[6]

1.3.3 Prioritisation based on SDGs

The SDGs are important criteria for prioritisation of actions. The expected development of the global population for example would prioritize the developing markets for construction, food and benign fertilizers. Linking chemicals to new technologies for solving future problems is a helpful approach. It is not recommended though to restrict innovations to a low number of selected key chemicals or even group of chemicals (e.g. solvents, pesticides).

1.3.4 Other prioritisation parameters

Further aspects relevant for a prioritisation of activities of the ISC$_3$ include the expected effectiveness of measures, technologies and (project and/or R&D) activities in terms of a rapid, efficient and effective implementation of sustainable chemistry and opportunities/possibilities for start-ups and SMEs to participate.

Both of these parameters correspond to the points discussed in 1.3.2, as emerging fields usually provide opportunities for entrepreneurs and new, more sustainable process or product innovations are more easily implemented in such emerging markets compared to traditional sectors such as bulk and petrochemistry.

[6] http://newscenter.lbl.gov/2014/08/18/bionic-liquids-from-lignin/

2 Petrochemicals and basic chemicals

2.1 Summary

Petrochemicals are high volume chemicals derived from crude oil or natural gas produced in amounts of 100 million tons and more per year. Primary products in the chemical tree include the olefins ethylene, propylene and the C4 stream (butadiene, isobutylene, butenes), the aromatics benzene, toluene and xylenes, and methanol. Follow-up petrochemicals are e.g. ethylene oxide, propylene oxide, ethylbenzene, cumene, acrylonitrile, formaldehyde etc. Basic chemicals in addition also include inorganic chemicals such as chlorine and caustic soda. In contrast to most fine chemicals and pharmaceuticals production petrochemical and basic chemical production is performed catalytically in continuous plants with high efficiency and high level of heat integration and automation. Energy efficiency and selectivity are real cost factors and plants are therefore highly optimized. Nevertheless process innovations are still possible, e.g. in terms of catalysts or improved reactors or downstream operations. Process intensification, i.e. the use of advanced heat exchangers, mixers, spinning disk reactors, high gravity (HiGee) separation technologies, or combinations like reactive distillations, heat exchange reactors and membrane reactors, can provide a step change in process performance, but is relatively difficult to implement in retrofits of existing plants. Other means include heat recovery and reuse and combined heat and power. Apart from breakthrough technologies, also continuous incremental process improvements on plant level have a relatively high impact on energy and feedstock demand, due to the large production capacity of petrochemical and base chemical plants.

However, higher impact, particularly with respect to GHG emissions, is expected from game changing technologies aiming at novel pathways utilizing alternative (low carbon footprint) feedstock. Focus of innovation activities is the use of either biomass or CO_2 as feedstock. The largest commercial area for biomass use is bioethanol in Brazil, which is used as fuel or further dehydrated catalytically to ethylene. Innovations take place in the use of second generation biomass, e.g. lignocellulosic biomass, could become technically available in the next years. The first plants demonstrating this technology are now coming into production, albeit with small capacities compared to current steam crackers. In addition to fermentation (ethanol) and transesterification (biodiesel), conversion technologies include thermochemical conversion to synthesis gas and pyrolysis to pyrolysis oil.

CO_2 can be used as a chemical building block, urea is a well known and by far the largest CO_2-based product in this regard. Demonstration plants are in operation for CO_2-based methanol (Carbon Recycling International CRI in Iceland) and for synthetic fuels from CO_2 and renewable hydrogen via syngas and Fischer-Tropsch synthesis (sunfire in Germany). Smaller demonstration activities exist for formic acid, and a large number of other processes is under investigation at lab scale.

In terms of sustainability, these pathways need to be carefully evaluated by LCAs and sensitivity/rebound effect investigations, as such pathways only comprise higher sustainability under specific circumstances: for instance, biomass routes should be based on 2nd or 3rd generation biomass to avoid food competition, and generally biomass-based routes often have a higher process energy demand. CO_2-based routes are likewise very energy demanding and require a reaction partner with high energy content, such as hydrogen. The latter has to be provided based on renewable electricity in order to end up with an advantageous carbon footprint.

Specific technical advances can be highlighted for individual petro- and basic chemicals. To mention just two: Catalytic fast pyrolysis (CFP) is suggested to be the most efficient and economically viable option for production of gasoline range aromatics, including benzene, toluene and xylenes (BTX), directly from raw solid biomass[7]. For chlorine production, the replacement of the mercury cell process by the membrane cell process is ongoing, recent developments include the use of bipolar membrane technology and the oxygen-depolarised cathodes (ODC) technology.

Table 3: Innovations in the petrochemical and base chemical sector

Innovation approach	Example
Process improvements	**Process intensification and other process improvements** • Process-intensifying equipment, such as novel reactors, and intensive mixing, heat-transfer and mass-transfer devices; • Process-intensifying methods, such as integration of reaction and separation, heat exchange, or phase transition, techniques using alternative energy sources, and new process-control methods.
Process improvements	**Heat recovery and reuse** • Total site pinch analysis, heat pumps, heat-absorption and cooling, Organic Rankine Cycles (ORC) • Heat exchange between companies in industrial conglomerates and (nearby) district heating.
Process improvements	**Heat source changes, renewables and combined generation of heat and power (CHP)** • Shift to low carbon fuels • Geothermal heat • CHP
Evolution of feedstock	**Bio-based feedstock** • Fermentation; e.g. bio-ethanol from lignocellulosic biomass(in some world regions careful investigation of social implications are necessary) • Transesterification, e.g. triglycerides conversion into biodiesel with subsequent use/valorisation of the by-product glycerol • Thermo-chemical conversion; e.g. cellulose gasification for the production of bio-methanol (BioMCN, 900 kt per demonstration facility) • Pyrolysis, thermal depolymerisation of biomass into pyrolysis oil, which can be fractionated into various high and low value products (LCA required)
Evolution of feedstock	**Utilisation of captured CO_2 as feedstock** • CO_2 with renewable energy sources to methanol, e.g. CRI demonstration plant, Iceland • CO_2 to synthetic Diesel via Fischer Tropsch; e.g. sunfire, Dresden, Germany

[7] T. Dickerson, J. Soria, Catalytic Fast Pyrolysis: A Review; Energies 2013, 6, 514-538; doi:10.3390/en6010514

Innovation approach	Example
Specific developments for selected chemicals	Aromatics • Catalytic fast pyrolysis of biomass Olefins • Methanol to olefin (MTO) process using green methanol (from biomass or CO_2 and hydrogen from renewable electricity) • Direct CO_2/H_2 conversion via Fischer–Tropsch to olefins (FTO) using modified Fischer–Tropsch catalysts (Synthol process by SASOL in South Africa) Chlorine • Membrane process and changing monopolar to bipolar membrane technology to save energy by minimising the inter-cell voltage losses • Oxygen-depolarised cathodes (ODC) technology

Source: Own compilation.

Biomass and CO_2 derived methanol and hydrocarbons (via Fischer-Tropsch) have wide implications for the decarbonisation of downstream sectors, in particular the transport sector. In addition to synthetic fuels that are comparable to today's fuels (synthetic diesel and gasoline) the development of tailored advanced fuels such as polyoxymethylene ethers (OMEx) is possible, which have superior combustion characteristics.

Production routes based on alternative feedstock will often need stronger collaborations with the agriculture sector (biomass), energy supply (renewable electricity) and other process industries (CO_2-utilisation). This requires intelligent material and energy flows in industrial symbiosis concepts.

The petro- and base chemicals sector is generally dominated by large enterprises, business opportunities for SMEs are rare.

2.2 Other points brought up by the Advisory Council

Whether or not one of the described pathways is truly sustainable should always be judged on a holistic (scientific, economic, social and environmental aspects) and a life cycle view.

The production of base chemicals from bio-based feedstock result in a number of by-products (not waste), that can be used as feed material, organic fertilizer or even bio-material in construction.

3 Polymers

3.1 Summary

Commodity polymers are manufactured in large production plants with capacities of more than 100 kilotonnes per year by means of continuous processes. Precursors are the basic petrochemicals, i.e. ethylene, propylene, BTX etc., major products are polyethylene, polystyrene, polyvinylchloride, polypropylene, polyacrylates, polycarbonates, polyols, polyamides and polyethylene terephthalate. Innovations comprise process improvements to yield the standard basic polymers or improved materials characteristics of existing polymers. Similar to the petrochemical sector, innovations mainly focus on changes of the feedstock base, i.e. the use of bio-based feedstock or, most recently, carbon dioxide. Several bio-based polymers have been commercialised, most of them however based on 1st generation biomass, in particular polyethylene from sugar-cane-based ethanol via ethylene in Brazil, though second generation non-food sugar based polymers are being developed in many countries in the world. Another example is polyethylene terephthalate (PET), partly produced using bio-based ethylene glycol (eventually from second generation non-food biomass) and p-xylene. The synthesis of p-xylene itself from biomass is possible from bioethylene in a four step process. A general drawback of routes like this is the degradation of highly functionalized molecules into simple structures with the high need of chemicals and energy.

CO_2 can be utilized as a feedstock in various polymerisation reactions, either by direct copolymerisation with CO_2 or indirectly by conversion of CO_2 derived compounds. Direct conversion of CO_2 includes for instance copolymerisation with propylene oxide (which is partly replaced by CO_2) to polyether polycarbonate polyols as precursors for polyurethane synthesis. Covestro has started operation of a 5 kt/year demonstration plant for this process in Dormagen, Germany in June 2016. An example of a CO_2 derived precursor for polymers is methanol produced from CO_2 and renewable hydrogen.

Valorisation of plastic waste streams, residue streams and recovery of end-of-life products is another important option. PlasticsEurope calls for zero plastics to landfill by 2025 as opposed to the 10 Mt per year of post-consumer plastic waste going to landfill in Europe today. This entails stimulating high-quality recycling and extended collection of post-consumer plastics as well as the use of efficient energy recovery for the post-consumer plastic waste that cannot be recycled in a sustainable way.

Three options for recycling of polymers can be distinguished: i) back to polymer (mechanical recycling), ii) back to monomer and iii) back to feedstock (breaking down polymers into hydrocarbons or a mixture of carbon monoxide and hydrogen by means of a thermal process).

As alternative polymers, either natural or synthetic bio-based polymers are used. Among natural polymers polyhydroxyalkanoates (PHAs), linear aliphatic polyesters, are an important class, they can in principle be used without modification for different types of final products: films, sheets, moulded articles, fibres, etc.

Examples of new bio-based polymers are poly-lactic acid (PLA), which is a compostable[8] compostable thermoplastic, but also suffers from low viscosity and brittleness, polyamide 11, a non-biodegradable polyamide biopolymer derived from castor oil, or poly-3-hydroxybutyrate (PHB), a polyester produced by a number of bacteria by fermentation with properties similar to polyethylene and polypropylene. Furthermore, PHB is an inert, biocompatible and biodegradable material which has been proposed for several uses in medical and biomedical areas.

Contrary to the commodity polymers, manufacturers of specialty polymers have to cope with a wide product variety and demand for customized polymers with tailored properties. Applications of specialty polymers are diverse, including: water treatment, paper processing, mineral sequestering, textile processing, personal care products, pharmaceuticals, drug delivery, petroleum production, enhanced oil recovery, coatings and inks additives, and sensors. Attention has to be given to reuse and recycling concepts for such materials. This is particularly challenging for compound materials.

Production processes for specialty polymers have enormous improvement potential and innovations target the use of continuous processes instead of batch-processing also for these small and medium volume productions. Table 4 provides an overview of the identified innovations in the polymer sector.

Table 4: Innovations in the polymer sector

Innovation approach	Example
Synthetic polymers from biomass	Polymer precursors from biomass: • Bio-ethylene made from bio-ethanol by catalytic dehydration

[8] according to EN 13432

Innovation approach	Example
	• Polyethylene terephthalate from bio-based ethylene glycol and terephthalic acid from p-xylene via carbohydrate fermentation to isobutylene or carbohydrate dehydration to furan intermediates • Polyacrylic acid can be produced from bio-based acrylic acid via 3-hydroxypropionic acid from glucose or glycerol or acrolein from glycerol • PEF : Polyethylene Furanoate • Bio-based polybutadiene
	Alternative bio-based polymers: • Poly-lactic acid (PLA) from renewable plant sources, such as starch and sugar • Polyamide 11 derived from castor oil • Poly-3-hydroxybutyrate (PHB) by fermentation of beet and cane molasses, corn starch, alcohols and vegetable oils • Bio-based polyhydroxyurethanes to replace polyurethanes • Biobased polybutadiene is another example having properties similar to natural latex/rubber.
Valorisation of waste, recycling	• Back to polymer (=mechanical recycling): Collection and mechanically processing of waste plastics to produce recycled polymers. • Back to monomer (=feedstock recycling): Breaking down certain polymers into their monomers by means of a chemical process. • Back to feedstock (=feedstock recycling): Breaking down polymers into hydrocarbons or a mixture of carbon monoxide and hydrogen by means of a thermal process.
Utilisation of CO_2 as feedstock for polymer production	Direct conversion of CO_2 • Biodegradable polypropylenecarbonates by conversion of CO_2 with propylene oxide for packaging films and sheets, resins, or shock resistant blends with polyhydroxybutyrate. • Polyether polycarbonate polyols as precursors for polyurethane synthesis.
	Polymers and polycondensates from CO_2 derived components • PE from conversion of CO_2-based methanol to ethylene and subsequent polymerisation • Sodium acrylate for polyacrylic acid from CO_2 and ethylene in a one-step reaction • Dimethylcarbonate as phosgene replacement for polycarbonates, polyurethanes
Improved specialty polymers	• Multidisciplinary approach to develop a fundamental understanding of the underlying structure-property relationships • Systematically vary the structure of functionalized macromolecules • Countless innovations; High-Temperature Polymers, Scavenger Resins, Fire-Resistant Polymers Synthetic Polymer Membranes, Liquid Crystal Polymers, Hydrogels and Smart Polymers, Electroactive Polymers, Dendritic Polymers, Shape Memory Polymers, Microencapsulation, Polymer Nanocomposites, Degradable Polymers , Polymerisation-Filled Composites, Ionic Polymers etc. Note: Resource use and end-of-life issues have to be assessed for each of these innovations:

Innovation approach	Example
Sustainable production of specialty polymers	• Flexible, modular production of water soluble speciality polymers in continuous plants • New catalytic systems to e.g. increase yields, more selectivity, etc.

Source: Own compilation

Specialty polymers offer large opportunities for value chain collaboration and business opportunities for small and medium-sized enterprises specialized in producing, customizing and processing polymers towards a given application.

3.2 Points brought up by the Advisory Council

There are manifold of examples not only for specialty polymers but also for commodity polymers where the contributions of polymers to downstream users are continuously delivering innovations; thinner packaging solutions, packaging solutions for longer food shelf life, packaging solutions for sensitive foods, active packaging, lighter cars, highly performing insulation materials, medical applications, sports equipment, etc…

It is the functionality and performance requirements of the polymer that often/mostly determine its sustainability contributions, for example: intelligent polymers for packaging material or durable polymer solutions for long life applications, medical applications etc… It is of course important to assess functionality in the context of environmental impacts (used raw materials, toxicity of ingredients). It is furthermore important to consider proper end-of-life solutions once the polymers cannot be sustainably recycled anymore. Innovation to depolymerize or chemical recycle mixed plastics in an economical and environmental friendly way should be considered part of the innovations for sustainable chemistry.

Polymers in consumer products should preferably be long-living, provided efficient recycling logistics are ensured or fulfill the criterion of full and fast mineralisation.

4 Agro chemistry (plant protection)

4.1 Summary

Agriculture plays a central role in achieving the SDGs, especially the goals 2 (zero hunger), 12 (sustainable consumption and production patterns) and 15 (sustainable land use). In his report to the UN General Assembly in August 2015, the Secretary-General pointed out the great importance of agroecology and organic and regenerative practices providing increased resilience through crop, animal and system diversification, crop rotation, permanent plant cover and significant underground carbon storage.[9] Following Hoffmann[10] a rapid and significant shift is needed "from conventional, industrial, monoculture-based and high-external-input dependent production towards mosaics of sustainable production systems that also considerably improve the productivity of small-scale farmers. The required transformation is much more profound than simply tweaking the existing industrial agricultural systems. However, the sheer scale at which modified production methods would have to be adopted, the significant governance and market-structure challenges at national and international level and the considerable

[9] United Nations, General Assembly: Seventieth session: Agricultural technology for development. Report of the Secretary-General. A/70/298, 6.8.2015.
https://documents-dds-ny.un.org/doc/UNDOC/GEN/N15/248/46/DOC/N1524846.DOCX

[10] Hoffmann, U.: Assuring Food Security in Developing Countries under the Challenges of Climate Change: Key Trade and Development Issues of a Fundamental Transformation of Agriculture. UNCTAD Discussion Papers No. 201, February 2011

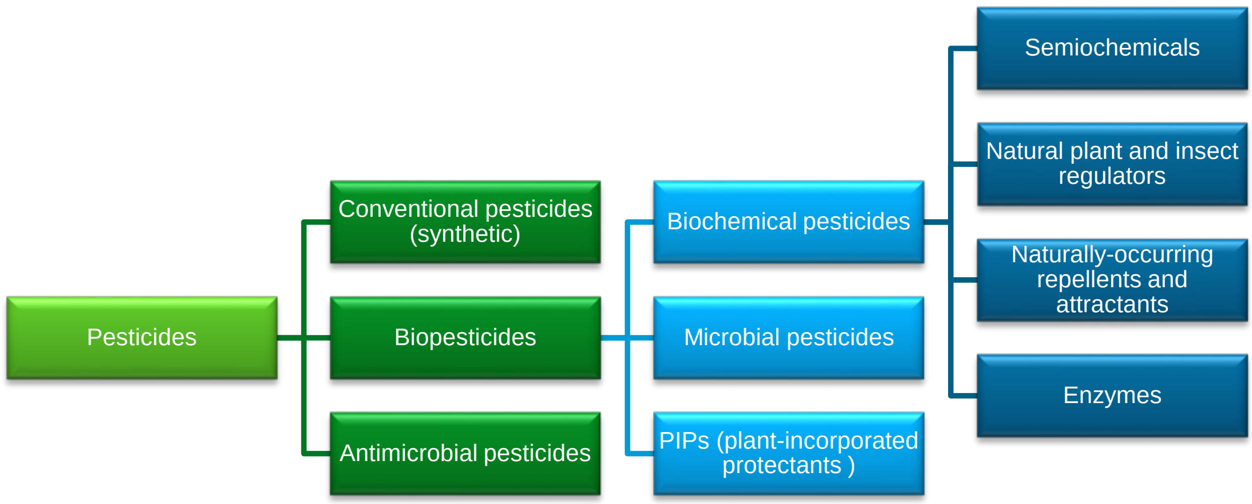
difficulties involved in measuring, reporting and verifying reductions in GHG emissions pose considerable challenges."

However chemical pesticides are one of the stabilising factors for the continuation of non-sustainable agricultural production methods. "Achieving targets 2.4 and 12.2 (sustainable production in agriculture) is directly dependent on successes in minimising the intensity of pesticide use. ... The implementation of targets 2.4 and 12.2 require a greater application of agroecological principles in agricultural production. For pesticides this means a return to the principles of *integrated pesticides* [correct is "integrated pest management"] with the concept of **"chemistry as a last resort"**. [11]

Within Integrated Pest Management (IPM) strategies, biological control agents (BCA) are regarded as most applicable in the context of appropriate preventative pest management. ASEAN[12] has grouped BCA into four product categories: (1) microbial control agents (microbials or MCA): bacteria and fungi, to a lower extent protozoa, nematodes and viruses, (2) macro-organisms (macrobials), acting as predators or parasitoids, (3) semiochemicals (mostly pheromones, kairomones, etc.), acting as attractants or repellents, (4) natural products (plant extracts or 'botanicals', fermentation and other products), including a wide variety of substances with different properties and biological activity.

The U.S. EPA, on the other hand, divides pesticides into three categories, one of them **biopesticides**[13]. These include naturally occurring substances that control pests (biochemical pesticides), microorganisms that control pests (microbial pesticides), and pesticidal substances produced by plants containing added genetic material (plant-incorporated protectants or PIPs[14]) (see Figure 1).

Figure 1: EPA: Pesticide categories



Own graph, based on EPA's website

Biochemical and microbial pesticides are subject to a different set of data requirements for registration than conventional chemicals. "Since biopesticides tend to pose fewer risks than conventional pesticides,

[11] German Environment Agency: Restart of the EU sustainability policy". June 2016, https://www.umweltbundesamt.de/sites/default/files/medien/1968/publikationen/160928_uba_position_eunachhaltig_englisch_barrierefrei.pdf

[12] ASEAN Guidelines on the Regulation, Use, and Trade of Biological Control Agents (BCA); ASWGC & BMZ/GIZ, 2014. www.asean.org/storage/images/Community/AEC/AMAF/OtherDocuments/ASEAN%20Guidelines%20on%20Biological%20Control%20Agents.pdf

[13] http://www.ecfr.gov/cgi-bin/retrieveECFR?gp=1&SID=39e02c5009b0e79c78490f0d27e32c22&h=L&mc=true&n=sp40.26.158.u&r=SUBPART&ty=HTML#se40.26.158_12060

[14] A list of PIPs is available under https://www.epa.gov/ingredients-used-pesticide-products/current-and-previously-registered-section-3-plant-incorporated

EPA generally requires much less data to register a biopesticide than to register a conventional pesticide. In fact, new biopesticides are often registered in less than a year, compared with an average of more than three years for conventional pesticides."[15] A list of biopesticide active ingredients registered in 2010 and earlier is available on the EPA's website[16].

In the **EU**, plant protection products in commercial form may only be placed on the market or used if they have been authorized (REGULATION (EC) No 1107/2009)[17]. Micro-organisms having general or specific action against harmful organisms or on plants, parts of plants or plant products, are regarded as 'active substances'. 'Micro-organisms' means any microbiological entity, including lower fungi and viruses, cellular or non-cellular, capable of replication or of transferring genetic material.

In the ASEAN countries (Brunei, Cambodia, Indonesia, Laos, Malaysia, Myanmar, Philippines, Singapore, Thailand, Vietnam) there are different national frameworks and a variety of numbers of registered products. Of the total of 471 registered products (as of October 2013), 296 were registered in Vietnam, followed by Indonesia (62) and Malaysia (46).[12]

Following Olson[18], biopesticides currently hold 5% of the total crop protection market (mainly in US, EU and Asia). This industrial segment is growing with a compound annual growth rate (CAGR) of 8.64%, a rate that is expected to continue through at least 2023. At that point the market will probably reach more than 7% of the total crop protection market ($4.5 billion, or more). Currently, approximately 75% of all biopesticides used worldwide consist of *Bacillus thuringensis* (Bt)-based products.

Biological control (including biopesticides) "is not universally appropriate for all pest management situations and there remains an evident and continuing role for chemical pesticides: nevertheless with an increasing proportion of natural products and their analogues."[12]

For a certain transition period, until a greater application of agroecological principles in agricultural production has been realized, it will presumably not be possible to dispense with the use of pesticides above all for pest infestation, see German Environment Agency's concept of **"**chemistry as a last resort".[11] These pesticides (active substances + auxiliaries) should pose only little risk to man and environment. The WHO Recommended Classification of Pesticides by Hazard[19] distinguishes between the more and the less hazardous forms of each pesticide in that it is based on the acute toxicity of the technical compound and on its formulations[20]. But, as the NGO PAN[21] points out concerning Highly Hazardous Pesticides (HHP): "Experiences in the past show that pesticides classified as only "moderately hazardous" by the World Health Organisation (WHO Class II) nevertheless give valid reason for concern. Examples are endosulfan and paraquat, pesticides that have caused thousands of poisonings, especially in developing countries, or pyrethroids which are known to cause various ill health incidences in the US. "A phase-out of and ban on HHPs have so far not been implemented. In addition and according to the Minamata Convention, the phase-out for pesticides containing mercury only applies from 2020 onwards, whereby exceptions continue to be allowed here too (Article 6).

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15 https://www.epa.gov/ingredients-used-pesticide-products/what-are-biopesticides

16 https://www.epa.gov/ingredients-used-pesticide-products/biopesticide-active-ingredients

17 http://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32012R0528&qid=1478681635346&from=EN

18 Sara Olson: THE BIOPESTICIDE MARKET. AN ANALYSIS OF THE BIOPESTICIDE MARKET NOW AND WHERE IT IS GOING. Outlooks on Pest Management – October 2015, 203-206. DOI: 10.1564/v26_oct_04 http://cdn2.hubspot.net/hubfs/86611/An_Analysis_of_the_Biopesticide_Market_Now_and_Where_It_Is_Going.pdf

19 WHO: The WHO Recommended Classification of Pesticides by Hazard. 2009. http://www.who.int/entity/ipcs/publications/pesticides_hazard_2009.pdf

20 Ia Extremely hazardous, Ib Highly hazardous, II Moderately hazardous, III Slightly hazardous, U Unlikely to present acute hazard

21 PAN International List of Highly Hazardous Pesticides (PAN List of HHPs). June 2015. http://pan-international.org/wp-content/uploads/PAN_HHP_List.pdf

Apart from biological (PAN: eco-system based alternative) solutions, active substances of conventional (synthetic) pesticides must therefore be developed which as far as possible fulfil the following **requirements** at the same time:

- Safe and fast effect on target organisms
- Low toxicity for humans and the environment
- Minimum effects on non-target organisms
- Good biological degradability
- No toxic, persistent or bio-accumulative degradation products, but fast and complete mineralisation
- No threat to the groundwater (no substantial substance intrusions into the groundwater)
- Low risk of selecting resistant biotypes by frequent use of agents with the same mode of action

In the agrochemicals (pesticides) industry, only a few innovative approaches could be identified. This is no doubt due to the fact that this is a very strictly regulated area (precautionary principle). However, it is also linked to the question of which role pesticides can/should play in sustainable agriculture and how innovations in this context should be defined, see the Report of the Secretary-General to the General Assembly of the United Nations[9].

With regard to pesticides there is a large number of sites of action in the target organisms, in the case of the pesticides used to date only a few modes of action dominate:

- Herbicides: Inhibition of EPSP synthase
- Insecticides: Nicotinic acetylcholine receptor (nAChR) competitive modulators and sodium channel modulators
- Fungicides: Respiration inhibitors, sterol biosynthesis inhibitors and multi-site action

In the period 1988 to 2009 (no newer data available), 47 new active substances were indeed developed. However, only three of them demonstrate a new mode of action (Mode of Action, MoA). The author ascribes this to the fact that all too often only "me too" concepts were pursued. In addition, in western industrialized nations, first and foremost the USA, industry has considerably reduced its research effort due to a concentration on GM seeds. The development of a new active substance for a new mode of action could therefore be considered as a real innovation in pesticide research. But US EPA's Multi-Year Workplan for Conventional Pesticide Registration[22] (as of September 14, 2016, based primarily on downloads from an electronic tracking system in the Office of Pesticide Programs (OPP)), includes only few registration requests for new pesticides (active ingredients) for non-food use, but mainly requests for new tolerances of already registered pesticides.

New active substances with well-known modes of action could also be considered an innovation within the meaning of sustainable chemistry if they display significant advantages over already established substances and independently of whether they resort to the one or other mode of action. In this way, active substances that work selectively in the case of intercropping, too, could lead to the reduced use of active substances. For the adjuvants needed, the requirements are the same as described before.

A real innovation would also be the identification, isolation and production of a biochemical or microbial biopesticide that is as far as possible species-specific. For example, Paul Stamets, mycology professor in the USA, has registered several patents on mycopesticides and mycoattractants since 2000[23]. However, research failed to reveal any corresponding large-scale use of SMART pesticides (Sporulating Mushrooms And Repelling Technology) in agriculture. And in the case of biopesticides too, attention must be paid to the entire lifecycle and the effects on non-target organisms. For example, *Beauveria bassiana* has – even if only in a very few cases – manifested itself as a human pathogen.

[22] https://www.epa.gov/sites/production/files/2016-09/documents/w2_webworkplanforposting_bychemical_newuses.pdf
[23] https://en.wikipedia.org/wiki/Paul_Stamets

Further innovations could exist in the combination of various active substances and/or auxiliary agents (to increase effect, for stabilisation, to form a stock etc.) of the optimisation of types of application.

However, whether for example a retard function through microencapsulation[24] of the active substance or nanopesticides (active substance is built into a small particle < 100 nanometers) can be regarded as an innovation within the meaning of sustainable chemistry can only be discussed under consideration of the **requirements** described above. In this way, it might be possible to reduce the amount of active substance dispensed by a substantial degree. On the other hand, nanopesticides can lead to further contamination of water and soil due to the improved transport and longer "lifetime" of the active substances. Microencapsulation of biopesticides for protection against UV radiation is a new, promising field of research.[25]

In the following section, a limited number of examples of innovations in the field of agrochemicals are presented, which could potentially support the objective of sustainable agriculture. With regard to the approaches presented, one has to keep in mind that these innovations need further input of materials and energy. Therefore an LCA approach is always necessary to clear the ecological advantageousness. In addition, an examination by independent third parties on the sustainability of these examples is not available.

Table 5: Innovations in the agrochemical industry

Innovation approach	Example
Biochemical pesticide / Microbial pesticide	**Bacterial nematicide substituting methylbromide** Since 2011 Syngenta and Pasteuria have had an exclusive global technology partnership to develop and commercialize biological products to control plant-parasitic nematodes, using the naturally occurring soil bacteria Pasteuria spp. A revolutionary in-vitro production process will enable the development of cost-effective nematicides with a novel mode of action. CLARIVA™ for control of soybean cyst nematode (SCN) and sugarbeet cyst nematode (BCN) is approved in several countries.
Biochemical pesticide / Microbial pesticide	**Biofungicide from soil bacteria** The active substance is a new strain of *Bacillus amyloliquefaciens*, which was isolated from a soil sample in the USA. It is reported to be effective in particular against downy mildew and other fungi and bacteria (including sclerotinia, macrophomina, eutypa, botrytis, rhizoctonia, and sclerotium).
Biochemical pesticide / Natural plant and insect regulators	**Biofungicide from giant knotweed** An extract of giant knotweed, *Reynoutria sachalinensis*, prevents and fights disease by triggering treated plants to produce disease-fighting biochemicals while enhancing plant health to optimize yield.

[24] BASF: Initium® – the innovative fungicide solution for specialty crops. http://www.agro.basf.com/agr/AP-Internet/en/content/solutions/fungicides/initium/index

[25] http://ecopesticides.net/#opportunity

Innovation approach	Example
Biochemical pesticide / Natural plant and insect regulators	**Water-soluble biopesticide based on neem**[26] Cold Pressed Neem Oil is registered by EPA as biopesticide active ingredient since 2009.[27] Dr. Yusup's team proposed to use a unique combination of different plant extracts to develop a water-based biopesticide. ... The bio-pesticide will be formulated using different plant extracts such as ginger, garlic, red chili and neem. The formulated product will be tested on paddy plants and should improve the productivity of paddy fields.

Source: Own compilation. An examination by independent third parties on the sustainability of these examples is not available.

5 Fertilizers

5.1 Summary

Apart from a considerable reduction and withdrawal in the long term from the use of pesticides and an exit strategy for particularly hazardous pesticides (see chapter Agro chemistry), the reduction of the use of mineral fertilisers is also on the agenda for various reasons:

The IAASTD report[28] sees enormous potential in resource-friendly land management: “Some "win-win" mitigation opportunities have already been identified. These include land use approaches such as lower rates of agricultural expansion into natural habitats; afforestation, reforestation, increased efforts to avoid deforestation, agroforestry, agroecological systems, and restoration of underutilized or degraded lands and rangelands and land use options such as carbon sequestration in agricultural soils, reduction and more efficient use of nitrogenous inputs; effective manure management and use of feed that increases livestock digestive efficiency”.[29]

In his report to the UN General Assembly in August 2015, the Secretary-General stated[30]:

“35. Improving soil health means going beyond singular applications of inorganic fertilizer. At a minimum, integrated soil fertility management involves the use of locally available resources, the combined application of organic resources and fertilizer, and more efficient use of both inputs. Where soil nutrients have been mined, more elaborate interventions are needed, such as subsoil tillage or the application of large quantities of high quality manure or lime. The availability of organic fertilizer can be enhanced by intercropping nitrogen-fixing legumes, such as pigeon peas or cowpeas, and nitrogen-fixing trees, such as *Faidherbia albida*. ...

[26] Neem is considered a weed in many areas, including some parts of the Middle East, most of Sub-Saharan Africa including West Africa and Indian Ocean states, and some parts of Australia. Ecologically, it survives well in similar environments to its own, but its weed potential has not been fully assessed. https://en.wikipedia.org/wiki/Azadirachta_indica

[27] https://www.epa.gov/ingredients-used-pesticide-products/biopesticide-active-ingredients

[28] Beverly D. McIntyre (ed.): Agriculture at a Crossroads. International Assessment of Agricultural Knowledge, Science and Technology for Development. Washington, D.C., Island Press, 2009.

[29] http://www.weltagrarbericht.de/reports/Synthesis_Report/Synthesis_9.html

[30] United Nations, General Assembly: Seventieth session: Agricultural technology for development. Report of the Secretary-General. A/70/298, 6.8.2015. https://sustainabledevelopment.un.org/index.php?page=view&type=111&nr=8396&menu=35

63. It is of critical importance to introduce agricultural practices that move beyond yield gains to build up organic matter in the soil. This will contribute significantly to mitigating climate change while also reducing soil erosion and increasing soil fertility and soil health."

Against this background, various sustainable chemistry approaches are conceivable for achieving the SDGs/a sustainable agriculture, in particular for a transition period until a complete changeover in agricultural production has taken place. In this context, new organic fertilisers, new or more effective processes for the recovery of nutrients (here above all phosphorus) from wastewater/waste, as well as a differentiated use of nutrient input or the development of optimized types of application for slower release and better plant uptake can be considered.

For phosphorus fertilizers, the problem of cadmium (Cd) contamination is another challenge. Technologies for reducing Cd content in mineral fertilisers are known for several years, but they were not practiced because of high costs and lack of demand (no legal regulations).[31] As the EU plans to tighten the limits for Cd in fertilizers, the situation in the member states has changed. Here, life cycle assessment for the different solutions is required. All the wastewater related recovery approaches have thoroughly to be assessed where, when and how they might be a sustainable contribution. Though called recovery technologies, only a (minor) share of nutrients can be won again (e.g. when P is recovered from effluents/sludge etc.). After that, it is spread out again onto the fields (dissipated) where only a part is taken up by plants (coming back to humans and into sewage again, a smaller part remaining in the plants residues left on the field), and some part of the (recovered) P is lost by leaching.

Some selected innovative approaches to the fertilizer industry are illustrated in Table 6. Approaches for the more efficient synthesis of ammonia are also of interest, cf. Table 6. With regard to the approaches presented, one has to keep in mind that these innovations need further input of materials and energy. Therefore an LCA approach is always necessary to clear the ecological advantageousness. In addition, an examination by independent third parties on the sustainability of these examples is not available.

Table 6: Approaches for innovations in the fertiliser industry

Innovation approach	Example
New organic fertilisers	**Biocoals** According to the World Bank, biocoal is likely to be suitable above all for small farmers in developing countries, since their fields would probably profit more from soil conditioners and because biocoal could be a key element for climate-smart agriculture. Considerable development work is, however, necessary to achieve this goal.
	Combination of humic acid and mineral fertiliser Under the aspect of innovation, the use of humic acid from ortho-lignite as a component of organo-mineral fertiliser to improve soil quality is certainly legitimate. However, leonardite, which is to be classified between peat and coal, is a fossil carbon source. Inspection of the overall system in terms of lifecycle assessment and climate impact (What actually happens to the humic fraction after separation?) would appear advisable.
Feedstock change	**Recovery of phosphorus from wastewater, sludge and ash**

[31] Cichy B., Jaroszek H., Paszek A., Tarnowska A.: Cadmium in phosphate fertilizers; ecological and economical aspects. CHEMIK 2014, 68, 10, 837–842. http://ec.europa.eu/DocsRoom/documents/2501/attachments/1/translations/en/renditions/pdf

Innovation approach	Example
	In industrialized countries with a good infrastructure for the collection and treatment of wastewater, appropriate measures should be taken to recover phosphorus. Processes to recover valuable substances from wastewater, sludge and ash have been available for years.
	Phosphorus enrichment and digestion of mineral residues containing phosphorus in liquid LD[32] sludge The project partners developed a process which produces a new, highly effective converter lime made of residues from burning sludge and meat and bone meal. Secondary phosphate carriers such as sludge ash are added to the liquid steel slag. Thermal digestion enriches the steel slag with phosphorus and removes heavy metals from the sewage sludge ash.
	Use of local sources of phosphorus In cooperation with Austrian design studio EOOS and Makerere University Kampala, Uganda, EAWAG (Swiss Federal Institute for Environmental Sciences and Technology) has developed the “Blue Diversion Toilet”.
More efficient use of nutrient inputs	**Slow release/controlled release, nitrification and urease inhibitors** When using fertilisers with urea, it should be noted that this compound, with the help of urease, an enzyme present in the soil, is converted into ammonium within two days. Using urease inhibitors (UI) blocks the enzyme’s activity. The period needed for conversion of urea to ammonium is slowed down, depending on soil temperature, by up to ten days.
Optimized application techniques	**Precision farming – Computer-Aided Farming (CAF)** Various technology providers offer solutions for the optimisation of fertiliser use, but also growth regulators or pesticides. The different crops are given exactly the amount of nutrients in each sub-area which is needed for them to reach their maximum yield capacity.
Optimized production techniques	**Biomethane as a source of hydrogen for the Haber-Bosch-process** One of the options to abate the carbon emission of ammonia production is to change the process of hydrogen generation. Hydrogen produced from other feedstock and (preferably waste) biomass is a particularly promising option. Biomass can be converted in a gasifier to produce methane that can be mixed with natural gas in ammonia production. It has to be kept in mind, that this is another competitor for biomass and a P-needing approach.
	Alternatives to the Haber-Bosch-process The recovery of hydrogen from water by means of electrolysis is a possible alternative source of hydrogen for to the Haber-Bosch-process. The technology was regarded as not economically feasible in particular due to the high energy costs leading to zero power at peak hours, but can become locally competitive, but can become competitive through the further development of renewable energies.

[32] Converter process according to the Linz-Donawitz method

Innovation approach	Example
	Minimisation of precious metal loss and greenhouse gas emissions in the production of nitric acid using the Ostwald process Complex catalytic converter systems have meanwhile been developed with which considerable savings in precious metals can be achieved. Further developments permit a reduction in the emission of nitrous oxide (laughing gas), the harmful greenhouse gas which is produced in small quantities as a side reaction in the Oswald process.

Source: Own compilation. An examination by independent third parties on the sustainability of these examples is not available.

Some new business models could also be identified, rarely, however, with links to other branches of industry. No examples were found for chemical leasing in the area of fertilisers. The focus here is more on the use of pesticides. An examination by independent third parties on the sustainability of these examples is not available.

Table 7: Business models along value chains

Innovation approach	Example
Value chain – Backwards	**Case study: N.V. Slibverwerking Noord-Brabant (SNB): P-recovery from ashes produced by mono-incineration of sludge** SNB and HVC currently incinerate around one half of the Netherland's municipal sewage sludge (c. 1.5 million tonnes/year). Because the companies use "mono-incineration" (sewage sludge incinerated separately, not mixed with municipal solid waste or other waste), the ash contains high phosphorus levels (up to 7% P). The project will recover over 4 000 tonnes/year of phosphorus.
	Case study: RecoPhos Consult GmbH: P-recovery from sewage sludge ashes With the RecoPhos® process, for which a patent has been registered, 98% of the phosphorus in sewage sludge can be recovered and fed back into the cycle. Less than 1% waste is produced when processing the ash to high-value phosphorus fertiliser. Questions related to contaminants and pharma residues may be still an issue.
	Case study: Remondis: REPHOS®-process for recovery of phosphate from waste water In the field of industrial wastewater treatment, REMONDIS Aqua has developed the REPHOS® process, with which phosphorus can be recovered directly from the wastewater stream in the form of MAP (Magnesium Ammonium Phosphate). The trick of this patented process is the fact that the MAP can be used directly in agriculture without any complicated dewatering process. However, the risk of repatriation of (organic) micro pollutants from wastewater in the ground via recovered phosphorus cannot be excluded.
	Case study: Ostara: Ammonia-Magnesia-Phosphate-fertilizer from waste water („Crystal Green") Struvite crystallisation and recovery is a promising technological process that has the potential to both remove efficiently phosphorus from wastewater by-products, and provide an alternative source of

Innovation approach	Example
	phosphate fertiliser. This technique is already applied commercially. However, the risk of repatriation of (organic) micro pollutants from wastewater in the ground via recovered phosphorus cannot be excluded.
Value chain – Forwards	**Case study: Polymer-coated controlled release fertilizers (CRF)** Polymer-coated controlled release fertilizers contain of water-soluble nutrients (e.g. NPK) that are wrapped in a flexible polymer membrane. Moisture can diffuse through this membrane so that a nutrient solution forms inside. This diffuses through the membrane to the outside at a speed which in the best case corresponds to the nutrient demand of the crop as it grows. The polymer membrane is biodegradable and decomposes within several months to CO_2, NH_4 and water (according to the manufacturer) and should preferably be plant-based. Polymer-coated CRF are offered by several companies, e.g. AGRIUM, ICL, COMPO or HAIFA.
	Case study: REMONDIS Aqua GmbH & Co. KG: Chemicals for the recovery of phosphorus for the production of high-quality phosphoric acid With the new process, sewage sludge ash is dissolved not, as usual, in hydrochloric acid, but instead in phosphoric acid, whereby the phosphoric acid is enriched with the phosphoric fraction of the ash and processed in various selection stages. In this way, phosphoric acid, amongst others, can be recovered for the production of phosphates (including fertilisers) and gypsum for the construction materials industry.
	Case study: BioCover AS: Optimisation of manure for agricultural use on sensitive soils (SyreN+) Application of animal slurry based on phosphorus value with adjustment of N-value through injection of liquid ammonia into slurry and eliminating ammonia emission through pH control using sulphuric acid, which doubles as S-fertiliser.
	Case study: Yara: TraP – Phosphorus trapping in soils and manure in order to maintain farming on vulnerable soils In the gypsum treatment of manure the dissolved phosphorus in slurry will settle onto the bottom of the slurry storage tank together with the solids. Sedimentation of dissolved phosphorus is achieved using a Gypsum-MgO-based precipitate, which is mixed with the slurry in the tank. Following treatment, the liquid fraction from the upper part of the tank can be spread on fields where phosphorus fertilisation is not required. The phosphorus-rich solid fraction can be transported to fields located further away where phosphorus requirements are often higher.
	Case study: BioEcoSIM In BioEcoSIM, an EU-funded project, the intention is to erect and operate a pilot plant in which pig manure is processed to organic soil conditioners and mineral fertiliser salts. BioEcoSIM will valorise livestock manure as an important example of valuable bio-waste into 1)

Innovation approach	Example
	pathogen-free, organic soil amendment (biochar), 2) slow releasing mineral fertilisers and 3) reclaimed water.

Source: Own compilation. An examination by independent third parties on the sustainability of these examples is not available.

6 Coatings, dyes, pigments and adhesives

6.1 Summary

The coatings, dyes, pigments and adhesives sector is complex and comprises many interfaces or overlaps with other sectors addressed by this study, e.g. specialty polymers, construction chemicals etc. The major change that has taken place in the coatings industry during the last 40 years has been the adoption of new coating technologies. Air pollution regulations will continue to be a driving force behind the adoption of new coating technologies. Despite the relatively slow growth in demand anticipated for coatings overall, waterborne and high-solids coatings, powders, UV curables, and two-component systems appear to have good growth prospects. In general, environmental regulations are becoming more stringent in all regions to limit emissions of volatile organic compounds (VOCs) and hazardous air pollutants (HAPs), not only in the industrialized world, but also in developing countries like China.

Additives belong to a broad and diffuse category of key components in a coating formulation. The focus on green technology, sustainability, nanotechnology, lower cost and safer products has led to the introduction of newer additives and chemistries, thereby still demanding the same or better performance than their traditional counterparts. Many of today’s additives are multi-functional; some are also incorporated into polymeric backbones. There are a number of new nano-sized additives and biobased additives in the market today; their functions are varied and they tend to overlap the past traditional categories.

The major avenues of production of “green” dyes are i) the extraction from plants, ii) the extraction from arthropods and marine invertebrates (e.g., sea urchins and starfish), the extraction from algae (e.g., blue-green algae) and the production from bacteria and fungi.

Innovations in the coating industry rely on work hand in hand with its upstream supplier networks that take materials from the ‘cradle’ and supply materials ready for formulation to the paint manufacturer’s gate. In designing the coatings of the future, the paint manufacturers must also understand downstream requirements of paints, their modes of application, the anticipated roles to be played by the coatings and the ways in which coated products are disposed of, once no longer required. To address this need, the chemical industry has organized a global supplier engagement program entitled Together for Sustainability (TfS).

Upstream innovations in the coating industry include the improvement of the raw materials footprint, either by replacing harmful ingredients or by using bio-based ingredients. Downstream, the development of recycling concepts (e.g. for waste paint or coated substrates) is necessary. Furthermore, paints and coatings providing enhanced lifetime and functionality are the main innovation areas. Enhanced functionality is a key area for product innovations which helps improving the sustainability of the downstream industry or the consumer application.

The sector is particularly suitable for innovations along the value chain, via joint and integrated collaborations with downstream sectors. Adhesives and sealants typically constitute only a small percentage of the final product they are incorporated into. In the majority of applications, the positive contribution made by adhesives and sealants can play a significant role in enabling the sustainability benefits of the product, particularly in terms of the substrates they are required to bond, the efficiency of the manufacturing process they are used on, the final end use of the bonded article, its durability and the opportunity to recycle the materials used at the end of its useful life.

Industry frequently brings innovation on coatings, dyes, pigments and adhesives to market, which address single aspects of sustainability such as energy efficiency. They have to be assessed carefully though with regard to other sustainability indicators. A few examples are listed in Table 8, including benefits and potential areas of concern.

Table 8: Examples for coatings and adhesives innovations and their impact

Innovation	Benefits	Critical aspects
Adhesives that replace or reduce the need for other fastening or strengthening systems.	• save energy during the manufacturing process; • consume less metal and plastic; and lead for example to lighter vehicles, which use less fuel and produce less carbon dioxide.	• check for toxic ingredients
• sealants in construction; sealing gaps between glass units and walls or walls and roof.	• use of insulating glass windows and facades helps minimise energy losses • UV and weather-resistant, require less maintenance and virtually invisible.	• check for hazardous ingredients • recyclability of materials and integrated products to be explored
• Replacement of metal/ plastic caps in automotive using eco-filters by specialised hot melt adhesives that are moulded to form adhesive caps which stick to the filter medium	• drastic reduction of weight improving fuel efficiency • rationalisation of the filter production process • advantages in the recycling process claimed	• check for hazardous ingredients • check environmental fate
• Flexible plastic packaging with layers of different plastics glued together with adhesives to protect food,	• Reduce food waste, keep it fresher for longer	• Efficient recycling needs to be ensured • Microplastic in oceans is of increasing concern
• Corrosion resistant coatings of base structure of wind power plants, adhesives for manufacture, maintenance and repair of long blades	• Improve lifetime and reduce maintenance (in particular offshore)	• check for aquatic toxicity • assessment of resource efficiency over lifecycle necessary

Source: own compilation

Table 9 lists a number of other innovations of the sector. As for the previous examples, caution has to be taken regarding sustainability evaluation here.

Table 9: Innovations in the coatings, dyes, pigments and adhesives sector

Innovation approach	Example
Technology innovations	• Nanoparticles in paints and coatings to increase scratch, mar, wear, corrosion, and UV resistance • Nanotubes for electrically conductive coatings and to increase the speed of reaction of thermosetting resins; • Organosilane dendrimer coatings • Buckyball coatings for machine parts • Metals for conductive coatings in inks
Bio-based ingredients	• Biobased polyvinyl ether copolymers for coatings, dyes, • Natural dyes
Enhanced functionality of coatings	• Internal and external roof coatings that reflect heat away from houses during hot seasons and keep warmth in during the winter; • Coatings that generate useable electricity; • Coatings that are scratch resistant in automotive applications; • Coatings that remove impurities from the air; • Low-emission paints to protect indoor air quality, particularly in well-insulated homes
Life cycle thinking	• Recycling of coated substrates and waste paint, • Design for recycle • Monitoring impact and sustainability advances
Substitution of hazardous ingredients	• Replacement of tributyl-tin (TBT) as marine antifouling agent

Source: Own compilation.

The coating industry provides high potential for value chain collaborations up- and downstream, as summarized in Table 10.

Table 10: Business models along value chains

Sector	Example
Value chain - Backwards	Collaboration with specialty chemicals and specialty polymer producers in the development of new coating substrates, additives, etc.
	Provide a bridging function between chemical/material providers and downstream sectors
Value chain - Forwards	Extend the functionality of coatings to enhance the sustainability of downstream products
	Support recycling concepts for downstream sector products and provide design solutions for better recyclability
	Engage in new business models such as chemical leasing

Source: Own compilation

7 Detergents, cleaning agents and personal care products

7.1 Summary

In Europe, hygiene standards are relatively high, but in many parts of the world hygiene is still an ongoing challenge. In the developing world, many lives are lost every day due to unsafe water, poor sanitation and poor hygiene. In the developed world, the emergence of certain infectious diseases in the home and public places indicates that there is room for improvement. Detergents, cleaning agents and personal care products not only fulfil important functions in order to satisfy basic human needs, but are also conducive above all to hygiene. The purpose of using them is to prevent possibilities for pathogens to multiply and cause infection and to make it difficult for them to enter the human body (e.g. skin care products) as well as to minimize toxic or sensitizing effects[33]. In societies in which efficient water supply, wastewater and refuse disposal are established, the risk of an infection with facultative pathogenic germs through lack of hygiene is negligible and above all down to the individual consumer's own behavioural pattern (this does not apply for obligate pathogenic germs). That is why – provided sensible hygiene principles are observed – it is generally not necessary to use microbicidal agents for washing laundry or basic or maintenance cleaning at home on a regular basis and/or on a wide scale. However, different standards apply for hospitals, care homes, hospices and lengthier infections (asymptomatic carriers) in the private sphere. In addition, for laundry detergents, the most relevant environmental impact results from the energy used to heat the water.

In countries where there is no or only an inefficient water supply, wastewater and refuse disposal, the situation is different. Here relatively harmless infectious diseases can quickly lead to a life-threatening situation due to poor nutrition, weak immune system, further infections, parasite infestation, unsafe water and poor sanitation. "We understand the goals of sustainable development can only be achieved in the absence of a high prevalence of debilitating communicable and non-communicable diseases, and where populations can reach a state of physical, mental and social well-being." [34]

Against this background, the question is what global function the chemical sector of detergents, cleaning agents and personal care products can have in the framework of sustainable chemistry. It can take on an important function here, since wellbeing is far from just a matter of the absence of pathogens. The demands placed on detergents and auxiliaries in countries where washing machines are standard are naturally different from those in countries where laundry is still washed by hand, for example in a tub. For this reason, the criteria presented below must be weighted differently depending on the addressee. Saouter (2011) answered the question "What makes a surfactant more sustainable?" as follows[35]:

- High and full biodegradability
- Low toxicity
- Data rich (not explained; presumably data exceeding the ones needed for registration/authorisation, e.g. LCA data)
- Not fossil based
- Based on renewable resources ...
  – but not impacting on deforestation, on water consumption and on biodiversity (see below)
- Produced as locally as possible
- High performance in product

[33] In sensitizing the immune system recognizes the allergen as an "enemy" and responds during the next contact with an allergic reaction.

[34] UN General Assembly: Resolution adopted by the General Assembly on 27 July 2012 [without reference to a Main Committee (A/66/L.56)] 66/288. The future we want. https://documents-dds-ny.un.org/doc/UNDOC/GEN/N11/476/10/PDF/N1147610.pdf

[35] Dr Erwan Saouter, Director Science & Environment (SARL), Geneva: WHAT MAKES A SURFACTANT SUSTAINABLE FROM AN EU ECOLABEL, LCA, OR REGULATORY PERSPECTIVE? CESIO, Vienne 8 Jun 2011

Regarding these requirements, the following aspects should be considered:

- While performing the LCA for detergents and cleaning agents for the EU Ecolabel, it has been recognized that the use phase has a significant impact on their environmental compatibility, since, apart from the composition, the dosage is decisive for the sewage load. Thus, in addition to the composition, the product design with regard to simple and economical dosage is a major influencing factor for the overall consumption[36].
- Cultivation of oilseeds for the production of "renewable" instead of petrochemical surfactants presumably causes automatically a loss of biodiversity due to the necessary cultivation areas. It is extremely important to take into account the cultivation of the raw materials, since monocultures and intensive agricultural use often lead to new environmental problems.[36] The NGO WWF has pointed out to this problem in a different context when replacing palm oil with other oil plants.[37]

Some of these requirements (e.g. produced as locally as possible) are likely to be weighted differently for various regions in the world. Overall, however, this approach appears to be helpful for further discussion. Detailed criteria (ecological, societal and economic, including life cycle assessment) are currently developed within a new European norm on Bio-surfactants and Bio-solvents (CEN: mandate M/491 for Bio-surfactants and Bio-solvents). These chemicals are based on biomass. "This calls for a thoughtful regulation of the parameters, which should be considered for the production of biorenewable chemicals, in order to avoid any direct conflict with food production."[38] On the other hand, e.g. the oil of underutilised tropical seeds can be used for the production of soaps.[39]

For the adjuvants needed (e.g. complexing and bleaching agents, enzymes, stabilizers, brighteners, activators, solvents) the requirements are (correspondingly applied) the same as described above. This is of special concern regarding e.g. disinfecting or conserving agents that come with the price of water pollution (micropollutants, may also hold for other personal care products and surfactants), or primary microplastics which include plastic pellets and plastic particles manufactured for particular applications, such as cosmetic products and abrasives.[40]

Several approaches for innovations could be identified in the industrial sector of detergents, cleaning agents and personal care products, cf. Table 11. With regard to the approaches presented, one has to keep in mind that these innovations need further input of materials and energy. Therefore an LCA approach is always necessary to clear the ecological advantageousness and avoid burden shifting - taking into account economic efficiency, social balance, environmental viability). In addition, an examination by independent third parties on the sustainability of these examples is not available for the most of them.

[36] Marcus Gast, German Environment Agency: pers. comm., 03.11.2016

[37] http://www.wwf.de/2016/august/kein-palmoel-ist-auch-keine-loesung/

[38] Bardhan, S., Gupta, S., Gorman, M. & Haider, M. (2015). Biorenewable chemicals: Feedstock, technologies and the conflict with food production. Renewable and Sustainable Energy Reviews, 51, pp.506-520. DOI: 10.1016/j.rser.2015.06.013

[39] Olubunmi Atolani, Elizabeth Temitope Olabiyi, Abdullateef Abiodun Issa, Hidiat Taiwo Azeez, Ehi Gift Onoja, Sulyman Olalekan Ibrahim, Marili Funmilayo Zubair, Olubunmi Stephen Oguntoye, Gabriel Ademola Olatunji: Green synthesis and characterisation of natural antiseptic soaps from the oils of underutilised tropical seed. Sustainable Chemistry and Pharmacy, Volume 4, December 2016, Pages 32-39, ISSN 2352-5541, http://dx.doi.org/10.1016/j.scp.2016.07.006.

[40] Kirsten Isensee and Luis Valdes, IOC-UNESCO: Marine Litter: Microplastics. GSDR 2015 Brief. https://sustainabledevelopment.un.org/content/documents/5854Marine%20Litter%20-%20Microplastics.pdf

Table 11: Approaches for innovations in the sector of detergents, cleaning agents and personal care products

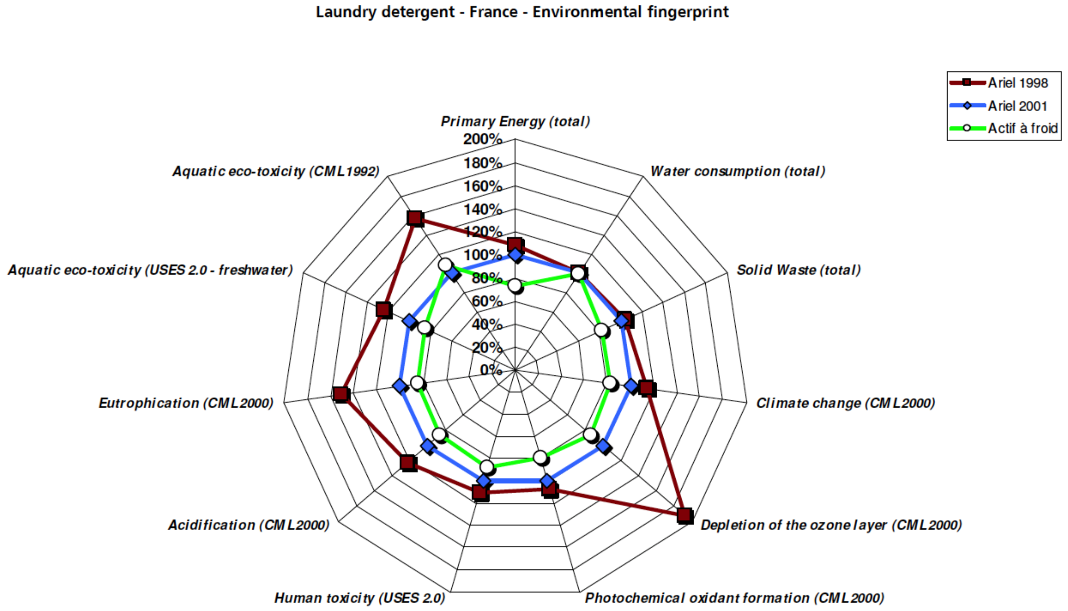
Innovation approach	Example
Biotechnology / Renewable resources	**Microbial biosurfactants** Biosurfactants belong to different substance classes, whereby the glycolipids (such as rhamnolipids and sophorolipids) make up the largest class. Sophorolipids are biosurfactants made by a fermentation process with a natural, non-GMO yeast using European sourced sugar and oil feedstock. The usage of sophorolipids makes it possible to increase both the ecological footprint and the performance of household cleaning formulations. The use of sugar could be an issue if sugar cane is used (e.g. high water demand in warm countries, labour aspects). Detailed criteria (ecological, societal and economic, **including life cycle assessment**) are actually developed within a new European norm on Bio-surfactants and Bio-solvents (CEN: mandate M/491 for Bio-surfactants and Bio-solvents).
Renewable resources	**Biobased sugar surfactants (Glucamide)** Glucamides are the foundation for new products for the market segments of personal care, industrial and home care, and crop solutions. Their environmental profile is excellent, with a high percentage of non-tropical biomass. For the use of sugar cane, see comment on microbial biosurfactants. Glucamide are used e.g. by Clariant. Its Glucamides are made from RSPO certified fatty acid esters or triglycerides (palm oil). [41]
Renewable resources / Residual biomass	**Bioethanol from agricultural residues** Major manufacturers of detergents and cleaning agents are cooperating with special chemical firms to expand the range of applications of bioethanol on the basis of agricultural residues, such as straw, for detergents and cleaning products (e.g. DuPont and P&G; Clariant and Werner & Mertz). On the other hand, the use of agricultural residues means that nutrients and structural materials are exported from the fields - that is of importance for fertility of soils.
Increased application efficiency	**Energy savings during washing by the introduction of enzymes (for example proteases, amylases)** Several companies have used consumer communications programmes, and broader calls to action at brand and industry levels, to encourage the use of colder temperatures. Manufacturers of detergents have partnered with suppliers to design technologies that provide greater performance in cold, and have also worked with A.I.S.E. on a major multi-stakeholder consumer education campaign to drive low-temperature washing (www.iprefer30.eu).
Production processes	**Resource-efficient production processes** Through controlled modification of the cultivation conditions of production strains of the *Pseudomonas putida* strain as well as combined expression of various genes of the rhamnolipid biosynthesis, rhamnolipids can be extracted which differ in their chemical properties and can therefore be used for different applications, e.g. as additives for cleaning agents, in cosmetics or for pharmaceutical applications.

[41] http://www.essentialingredients.com/pdf/GlucoPureBrochure.pdf

Innovation approach	Example
	NOTE: In Germany, according to the legal framework (§ 5 (1) GenTSV combined with Annex I GenTSV), Pseudomonas putida is classified as a donor and recipient organism for genetic engineering in risk group 2.[36]
Improvement of the entire life cycle	**Improvement in environmental indicators based on the entire life cycle** In the framework of an LCA study, it was possible to prove that the introduction of a washing detergent, which produces a comparatively good washing result at low temperatures, demonstrated better results than predecessor products for a total of 11 environmental indicators (Figure 1). Life cycle thinking is also the basis to lower the sustainability footprint of detergent products, e.g. via 'Advanced Sustainability Profiles' of products in the context of the A.I.S.E. Charter for Sustainable Cleaning (established in 2005).

Source: Own compilation. An examination by independent third parties on the sustainability of these examples is for most of them not available.

Figure 2: LCA results for a washing detergent



Source: Procter & Gamble 2006. http://www.jmu.edu/EnvironmentalMgt/Courses/ISAT422/Supplements/Laundry%20Soap%20LCA.pdf

Table 12 depicts aspects of value chain integration and business models in the sector of detergents, cleaning agents and personal care products.

Table 12: Approaches for new business models in the sector of detergents, cleaning agents and personal care products

Approach	Example
Value chain - Backwards	**Strategic partnerships with producers of biorenewables** The Du Pont example of extracting bioethanol from cellulose instead of maize is marketed under the name "Tide Cold Water "powered by nature". Other manufacturers of surfactants have already entered into strategic partnerships with producers of biorenewables, both up-stream and downstream.
Value chain - Forwards	**Producing "what's needed, when needed, where needed"** The F³ Factory programme[42] has been a unique collaborative endeavour that could stimulate the transition to a new business model for the whole chemical sector. In this new model flexible, modular, continuous and intensified technologies are used to meet the challenge of producing "what's needed, when needed, where needed" therefore minimising the environmental and economic footprint and reducing business risk.

Source: Own compilation.

8 Chemical fibres

8.1 Summary

The main function of fibres is to carry load along its length (not across its width) providing strength and stiffness in one particular direction. Fibres can be placed with a specific orientation (typically 0º, +/- 45º or 90º) to provide tailored properties in the direction of the loads applied. As a result, the mechanical properties of most FRP composites are considerably higher than those of un-reinforced resins.

The demand for fibres for clothing as well as technical purposes is growing disproportionately to population development. The total global production of synthetic and natural fibres is almost 100 million tons, whereby production of synthetic fibres has greatly increased and meanwhile accounts for half of total production. Through the high surface intensity and the high water demand in the case of cotton, further growth for fibres made from natural materials is limited.

In the chemical fibres sector, numerous approaches for innovations in the direction of sustainability could be identified. It can be seen in the production processes that waste and water-intensive processes, such as pulp or cellulose manufacture, can be converted to almost completely closed production cycles. In the case of conventional processes, it is apparent that more and more waste products can be used as raw materials in other areas, e.g. for the synthesis of platform chemicals. The use of ionic liquids offers considerable possibilities for the production of certain intermediates or commodities from biomass, meaning that the material use of lignin is just around the corner.

With regard to innovative applications and new fibre materials, the focus is partly on sustainable development in other areas (e.g. greater energy efficiency) and partly the sustainable innovations are related to the actual material itself. As examples of innovative materials, which moreover demand completely new synthesis methods, the following should be mentioned: Nanocrystalline cellulose, spider silk and partly also the "tailormade" fibres, which are produced from special polyamides including types based on castor oil. New types of composites are to be found above all in fibre-reinforced polymers, where by using selected natural fibres as a substitute, e.g. for steel, energy demand in production can be reduced

[42] http://www.f3factory.com/scripts/pages/en/home.php

or access to a reproducible raw material is regarded as a step towards more sustainability. The outcome is some interesting properties, but on the other hand the tensile strength of steel or aluminium-reinforced polymers is often not achieved. Another interesting development, which is aimed at lengthening the service life of fibre-reinforced polymers (composites) in the construction sector, is “self-healing” materials.

Synthetic fibres can also be produced on the basis of natural raw materials or from suitable types of waste. There is a range of niche applications in the paper and cardboard industry, where cellulose is either replaced or supplemented by fibres from vegetable waste.

Numerous studies deal with a substitution for the production of carbon fibres, which is material and energy-intensive, through synthesis from lignin or the use of carbon fibre waste from composites for re-use.

In Table 13, a number of innovative approaches for sustainable chemistry in the area of fibres are presented. The field of chemical fibres is so vast that the developments and case studies identified during research work only partially describe it, but are likely to be representative for development trends.

Table 13: Approaches for innovations in the field of fibres

Innovation approach	Example
Production process	Synthesis of important base chemicals (e.g. levulinic acid, triterpenes) from waste from the cellulose or paper industry
	Cellulose fibres from pulp in an almost closed production cycle using N-methylmorpholine oxide (Tencel® process)
	Nanocellulose from biotechnological processes (white biotechnology)
	Use of ionic liquids to break down various types of biomass as far as lignocellulose, including their use to break down cellulose at room temperature and to insert functional groups into the molecular structure of the cellulose
New materials or fibres/products with innovative properties	Combination of cellulose with fibres from other natural products (mostly woody waste from plant stems or fruit husks) as a basis for special types of paper and cardboard
	• Nanocellulose products: • Microfibrillated cellulose (MFC), amongst others for emulsion and dispersing agents due to high water storage capacity and increase in tensile strength of composites. Industrial application • Nanocrystalline cellulose (NCC), amongst others for tear-resistant transparent films, flexible displays and very light and stable aerogels (as structural elements and for thermal insulation). Conjugation of nanocellulose with polyaniline for ion transport in very thin polymer matrices (accumulator technology) • Bacterial nanocellulose (BNC) for extremely high-strength nanofibre networks (including applications in medicine for microimplants) –no industrial production so far
	“Tailormade” fibres on the basis of specially synthesized polyamides (e.g. polyamides from C11 – C18 dicarboxylic acids on the basis of castor oil and diamines, e.g. Terryl®, made from pentamethylene diamine out of sugars)

Innovation approach	Example
	Fibre-reinforced polymers (FRP) with “self-healing” properties, which are based either on a vessel system, which releases corresponding substances (e.g. low-viscosity epoxy-based resins) to repair cracks, or on reactive groups, which are attached to different molecular strands in the material and react with each other in the event of damage to create new bonds
	Spider silk: By contrast to nylon or Kevlar both stable as well as elastic, fully biologically degradable; batch synthesis through genetically modified bacteria (pilot production)
	Substitution of steel, aluminium, synthetic organic fibres, glass fibres, carbon fibres in composites (e.g. in polyester) through natural fibres (jute, kenaf, hemp…) to achieve a considerably lighter material with the same stability (energy saving in vehicle construction), whereby natural fibres are still used where technological requirements are less demanding
Change of raw material base	Production of carbon fibres from lignin rather than through pyrolysis of polyacrylonitrile or pitch, allowing access to a far cheaper natural material (not yet usable on an industrial scale)
	Use of polyols (waste products from production of biodiesel or of soya oil) in place of oil-based polyols for chemical syntheses
	Use of agricultural waste with fibrous structures for production of construction materials (see section on construction chemicals)
	Use of bamboo fibres in cement for high tensile strength with lower specific weight (see section on construction chemicals)
Process improvement	Optimisation of injection-moulding process for natural fibre-reinforced polymers (NFRP) due to lower thermal resilience of natural fibres during processing, in parallel also for NFRP based on biopolymers (PLA, PHB…) to ensure required material properties (e.g. crystallisation behaviour, heat deflection temperature, mechanical properties)

Source: Own compilation.

Fibre products used in construction are discussed in the chapter on “Construction Chemicals”.

It can be seen from the list that the desired result in the case of many of the products named can only be achieved through cooperation between the chemical industry and downstream stages in the value chain. The high complexity and wide variety of options especially in the area of composites lead to stronger cooperation between different industrial sectors and also to other sectors entering “classic” production in the chemical industry, such as the pulp and paper industry. Added to this are partnerships between small enterprises specialized in biotechnological processes or the treatment of otherwise unused natural materials either with the chemicals industry or with interested manufacturers of end products. This partly also includes the provision of seed capital.

In addition, opportunities exist for enterprises with access to waste as well as know-how in the area of separation and treatment processes. With regard to economically interesting materials, such as waste from carbon fibres or carbon fibre composites, there are many projects for the recovery of reusable materials, which represents a major challenge especially in the case of composites and has so far only led to gradual downcycling. Whilst it is a matter here of small volumes with high value added, the recycling of textile fibres for the clothing industry has long played a more important role. In this mass market, new business models are emerging which are likely to be driven by marketing, but could also bring with them a more sustainable use of clothing textiles.

Examples are presented in Table 14.

Table 14: Business models along value chains

Sector	Example
Value added chain - Backwards	Optimisation of production, use and re-use of fibres as further development in the pulp and paper industry (strategic approaches, amongst others supported by the association of the European fiber and paper industry (CEPI)) Taking back of used textiles by retail chains in the clothes sector
	Taking back by retailers only of textiles produced or sold themselves as voluntary individual manufacturer responsibility
	Recovery and re-use of carbon fibres from composites
Value added chain - Forwards	Optimisation of production, use and re-use of vegetable fibres as further development in the pulp and paper industry Increase in the use of biopolymers for specific purposes (e.g. BPA for agricultural foils)
	Biorefinery concepts (see chapter on “Petrochemicals”)
Marketing	Push-pull marketing as market development strategy right through to end customer to communicate new possibilities (push) and identify new customer requirements (pull) without entering the intermediate stages of the value chain

Source: Own compilation.

9 Construction chemistry

9.1 Summary

The “construction chemistry” sector is complex and demarcation is difficult. Looking at “construction chemicals”, such as adhesives, coatings, paints, wood preservers, fillers etc., does not go far enough – it is not possible to erect a building just with these. (Construction of infrastructure was excluded from the survey). For this reason, construction materials must also be considered in terms of their quantitative importance, whereby topics such as resource management, energy consumption and emission of greenhouse gases (GHG) and hazardous properties form an interface here to Sustainable Chemistry. When selecting construction materials for the building envelope as well as for its interior partitioning, regional and cultural backgrounds play a significant role. Approaches to Sustainable Construction can therefore be assessed differently from region to region, as they are dependent, amongst others, on the local availability of suitable materials, and the long-distance transport above all of construction materials leads to considerable energy input. “Sustainable Construction Chemistry” currently plays only a minor role in the discussion on construction and buildings. A wide spectrum of criteria for “sustainable construction” can be found in the large number of “Green Building Rating Systems”. Essentially, these are:

- Durability of the building
- Lifecycle costs, if available

- Specific energy consumption of the building (during construction, in terms of its ecological ruck-sack, during the utilisation phase)
- Use of reproducible raw materials
- Use of recycled material[43]
- Dismantling possibilities, including recycling of construction materials
- Construction chemicals used, amongst others with regard to their toxicity, handling and pro-cessing problems etc.
- Quality of indoor air.

In some cases, these systems, like norms or procurement rules in the public sector too, take into consid-eration the topic of construction chemistry only to a minor extent and differ from region to region.

In the area of construction materials, numerous successful approaches can be seen with which far lower GHG emissions in the production of cement and its processing to concrete can be achieved. Different routes are taken here:

- Energy saving in cement production through process optimisation
- Use of waste products (partly with a renewable materials fraction) to heat cement furnaces
- Substitution of $CaCO_3$ with industrial waste and natural pozzolans with low CaO fraction
- Use of recycled concrete flour as substitute in concrete production.

The level of progress in these approaches differs depending on the region. Further innovations, both for construction methods as well as with regard to energy saving and reduced GHG emissions, are being created by lightweight concrete, where many recipes are already available. Developments in lightweight concrete go as far as Ultra High Performance Concrete, where nano-silicic acid is used, which through better nucleation during setting results in a concrete far lighter than conventional types of concrete with the same strength, rigidity and load-bearing capacity. Precise control of setting, amongst others with the objective of faster hardening with as high a level of homogeneity as possible, in turn leads to a demand for special chemicals.

In view of the energy demand for heating and cooling, the development of insulating materials plays an important role. This was examined in greater depth for the following reasons:

- The energy/climate/chemistry interface plays a decisive role and the outcome is an important innovation driver
- Very different basic chemical building materials are used
- Materials from renewable as well as non-renewable sources are used
- The type of insulation and the input materials are important for indoor air too.

Polystyrene (EPS, XPS), polyurethane, rock wool, glass wool and similar products have been on the mar-ket for a long time as a "second building envelope", but they only achieve heat transition coefficients of at most 40 mW/(m x K). An improvement in the insulating properties of polystyrene can be achieved with a finer foam. The goal is far thinner wall thicknesses and better insulation up to < 4 mW/(m x K). Materials such as aerogels and evacuated open-pored materials which achieve about 10 mW/(m x K) are already used in technical applications. Development work is moving in the direction of insulating

[43] Potential problems caused by the recycling of materials including hazardous chemicals are not discussed in the Rating Systems investigated. Obviously, this issue has not been recognized by the responsible persons in this field.

materials with pores < 100 nm, which are filled with air or better with inert gas, whereby heat transition is virtually nil in the case of pores < 10 nm.

The energy/construction materials interface also plays the most important role in phase-change wall panels; these should serve as latent heat accumulators or temperature controls for building interiors.

The lifetime of structural building components can be extended if these have “self-healing properties” in the event of crack formation. There is a broad range of additives which are added to the concrete in the form of microcapsules, including polymers which can close a cracked bond by forming a new homolytic or heterolytic bond. Supramolecular polymers with non-permanent reversible bonds are currently being developed.

The narrower field of construction chemistry has many interfaces with the topics of indoor air and occupational safety. Amongst others, wood protection plays an important role. In addition to a large number of biocides which have mostly been available on the market for many years and passive wood protection, a few newer approaches (drying of wood with the aim of preventing rot by physical means, prevention of the ageing process of wood coatings by means of nano ZnO) can be mentioned as potentially sustainable alternatives or additions. Adhesives, fillers etc. used in construction contain large amounts of solvents or react with each other when used (e.g. in-situ foam) or with the air (e.g. cross-linked polymers). The substances released in the process can present a considerable occupational safety problem and are additionally still measurable over a long period inside rooms, where they can potentially trigger a chronic effect. It was not possible to sound out the large number of substance groups used here. Examples show that innovations are also initiated through occupational safety in order to avoid endangering construction site workers.

The substitution of non-renewable raw materials with renewable alternatives plays a major role, whereby many innovative applications are still at the research stage or in the pilot phase. In addition, it is here that the regional availability of suitable substitutes plays an important role. In general, the use of fibres from hemp, jute or flax for insulating purposes is possible, whereby the physical properties so far do not always match the quality of synthetic materials. An insulating material from fungal mycelium is being produced on an industrial scale in the USA. Regional sustainable solutions can result from the recycling of crop residues, which are otherwise treated as waste, for use as base material for insulating materials or as an additive for MDF chipboard as a wood substitute, depending on their physical properties. Ash from the incineration of sugarcane bagasse is suitable as pozzolan additives for cement. Thanks to their excellent tensile strength, bamboo fibres can be used to stabilize concrete constructions. Moreover, natural substances can be used in composite panels for insulating purposes. Which approaches are put into practice naturally depends on the cost benefits achievable in comparison to conventional materials and national regulations regarding the approval of construction materials.

The use of wood or also suitable types of earth as building material is mostly a regionally determined phenomenon; however, the use of wood for construction purposes is evidently also increasing in some countries outside traditional wood construction regions (e.g. Scandinavia).

A number of innovative approaches for the construction chemistry sector overall are presented in Table 15. In view of the breadth of the subject, only a selection is described here. This reflects more or less development trends in industrialized countries. It was not possible within the time period set to gain an overview of the abundance of traditional and new (potentially sustainable) approaches in emerging and developing countries.

Table 15: Approaches for innovations in the construction chemistry sector

Approach	Example
Production process	Reduction of GHG emissions in the production of cement (use of alternative energy sources, substitution of $CaCO_3$ with industrial waste and

Approach	Example
	natural pozzolans, greater energy efficiency of the process, recycled concrete)
	Foaming agent for PUR with lower GHG effect
	Energy-saving production of styrene (polystyrene) from ethyl benzene (see section on “Polymers”)
New materials or products with innovative properties	Infra-lightweight concrete < 800 kg/m³ with good thermal insulation properties (high percentage of fine-grain materials – “Microsilica”)
	Lightweight geopolymer concrete on the basis of aluminosilicates or blast furnace slag plus liquid glass; further development to ultra high performance concrete by adding nano-silicic acid
	Thinner insulating panels from polystyrene by producing smaller pores
	Development of new insulating materials based on aerogels, vacuum technology, nano pores on the basis of silicic acid with a target value of 4 mW/(m x K)
	Insulating foams on the basis of fungal mycelium
	Insulating foils for window panes to reduce solar radiation by about 50%
	Latent energy storage through phase-change wall panels with the aid of salts with high specific crystallisation energy enclosed in microcapsules
	Wood protection through complete drying of the wood to prevent rot with the aid of high-frequency waves (induction of electric dipoles leading to heat dissipation)
	Prevention of ageing of protective coatings on wood by adding nano ZnO
	Construction materials with “self-healing” properties (concrete through subsequent water absorption and setting of non-hydrated cement particles; polymers with the possibility to form new homolytic or heterolytic bonds; currently under development: supramolecular polymers)
Change of raw material base	Insulating materials based on reproducible raw materials (plant fibres)
	Composite panels for insulation purposes using reproducible raw materials (“ECO Sandwich”)
	Waste from crop residues (cotton stems, coconut fibres, rice straw, maize plants, sugarcane bagasse, bamboo fibres) as raw materials for use as or in construction materials
	“Organic dowels” from bio-based polyamide 6.10
	Wood as raw material for structural building components
	Chipboard with additives based on plant waste
	Earth as construction material

Source: Own compilation.

Desk research did not reveal any major shifts in business activities along the value chain. This is not, however, proof that no such developments are taking place in individual cases.

In the area of marketing, advertising for buildings and construction materials which makes reference to their “natural” origin, such as materials from plant parts, wood construction etc., is common.

The development of chemically very complicated materials or additives for complex reactions with the need for numerous tests requires cooperation between manufacturers of construction materials and producers of suitable additives. This applies even more so for construction chemistry products such as adhesives, sealants, protective coatings, plasters and screeds. Increasing complexity and higher functional requirements will lead to the relationship between the manufacturers of construction materials and of construction chemicals, which has mostly already existed for a long time, becoming even closer.

Table 16: New business models

Sector	Example
Marketing	Advertising with “natural materials”
Cooperation	Supramolecular materials
	Substitution of concrete additives

Source: Own compilation.

10 Pharmaceuticals

10.1 Summary

For the pharmaceutical industry, several areas of innovation can be pointed out in the context of sustainability. In accordance with SDG3 (Good health and well-being), the development of novel drugs is an important priority. This includes the development of affordable medication to treat diseases such as malaria, tuberculosis or HIV/AIDS, but also rare diseases for which often few or no drugs are available. There are approximately 7,000 different types of rare diseases and disorders, with more being discovered each day. However, only a small subset of new approved drugs is novel drugs. About 47% of the novel drugs approved in 2015 worldwide (21 of 45) were approved to treat rare or “orphan” diseases. Other new pharmaceuticals contribute to quality of care, greater access to medication, more consumer choice, and a competitive marketplace that enhances affordability and public health. Research is also required for the identification of new drug targets.

Drug delivery is another strong innovation field. Many different systems are investigated to deliver drugs at controlled or slow rate or in a more targeted manner, e.g. overcoming biological barriers. Excipients play a crucial role in the drug delivery systems. Some of them may be more sustainable than others. For capsules, oxygen permeability is important. Low permeability prevents oxidation of the active ingredients, resulting in a longer shelf life. The choice of the hydrocolloid in the capsule manufacturing is also guided by the dissolution profile: for quick release high dissolution profiles are needed. The optimisation of the excipient choice in the manufacturing of tablets/capsules is also important to prevent rejections (waste).

A key innovation area for the pharmaceutical industry is the use of the Green Chemistry principles to develop atom-efficient and more benign synthesis strategies for synthetic steps widely used for pharmaceutical manufacturing. Typical E-factors representing the ratio of waste to product (kg/kg) in the pharmaceutical industry are at 25-100. The ACS GCI Pharmaceutical Roundtable conducted a survey that identified areas in need of focused research to advance the principles of green chemistry and their application in the pharmaceutical industry. Ten chemical transformations and two process related operations were identified and published.

Likewise, pharmaceutical companies identified the main engineering challenges in pharmaceutical production. Manufacturing of active pharmaceutical ingredients (API) today is predominately performed in relatively inefficient batch processes. Hence, process innovations driven by the Green Chemical Engineering principles include e.g. continuous processing with intensified equipment, integration of reaction and separation steps and rationale solvent selection. The integration of primary (API) and secondary (formulation of drug) manufacturing is another area of investigation for large pharma companies.

Finally, the fate of pharmaceuticals in the environment is an area of concern. This requires benign-by-design synthesis strategies for pharmaceuticals, but also management strategies for pharmaceutical waste and water/wastewater treatments to eliminate drug residues. Table 17 provides an overview of the innovation fields.

Table 17: Innovation fields for the pharmaceutical industry

Innovation Approach	Example
Novel drugs	• New dosage forms, cost-saving generic formulations contributing to quality of care, greater access to medication and a competitive marketplace that enhances affordability and public health • Development of “orphan” drugs for rare diseases for which no medication is currently available • Development of dedicated drugs for children
Drug delivery	• Beaded delivery formulations to achieve long-acting drug levels • Colloidal carrier systems for pulmonary drug delivery, micellar solutions, vesicle and liquid crystal dispersions, nanoparticle dispersions • Nanoparticles as carrier crossing biological barriers
New synthesis strategies allowing for lower waste generation and higher atom economy	Amide formation avoiding poor atom economy reagents, e.g. using enzymatic catalysis, and use of boric acid to catalyse amide formation
	• Alcohol activation for nucleophilic substitution; e.g. catalytic activation of allylic and benzylic alcohols, or with amines by in situ oxidation and reduction catalysed by iridium complexes • Reduction of amides without hydride reagents; hydrogen is the ideal reductant because the only byproduct is water.
	Oxidation/epoxidation without chlorinated solvents; molecular oxygen as ideal oxidant; hydrogen peroxide as second best choice, sodium hypochlorite as one of the most economical oxidants.
	Greener Mitsunobu reaction (condensation reaction of alcohols with compounds having an active hydrogen), ideally catalytic in nature, with the stoichiometric oxidant and reductant generating innocuous by-products; e.g iodosobenzene diacetate as the stoichiometric oxidant, producing the more benign byproducts acetic acid and iodobenzene, instead of hydrazide
	C–H activation of aromatics; direct activation of aryl hydrogen for metal-catalysed crosscoupling reactions such as Suzuki–Miyuara; with proper catalyst recycle concepts
	Asymmetric synthesis • of aliphatic amines; direct reductive amination from prochiral ketones • Asymmetric hydrogentation of unfunctionalised olefins/enamines/imines
	New greener fluorination methods, catalysts for increasing the nucleophilicity of F_2, milder conditions for conducting fluorine exchange reactions, safer and more economical sources of electrophilic fluorine.

Innovation Approach	**Example**
Engineering innovations	Note: fluorine is generally a challenge after excretion of the fluorinated drug into the environment (low biodegradability)
	"Hydroxyl to amine'' transformation avoiding azides and hydrazine; alternative nitrogen nucleophiles
	Replacements for dipolar aprotic solvents with human reproductive risks, N-methylpyrrolidin-2-one (NMP), N,N-dimethylformamide (DMF) and N,N-dimethylacetamide (DMAc)
	Solvent-less reactor cleaning, e.g. high-pressure water jet technology, efficient detergents
	Continuous production instead of batch processes
	Intensified, more energy efficient separation methods and integrated reaction-separation
	Bioprocesses and biotransformations to enable highly stereo-, chemo-, and regioselective routes, reduce the number of synthesis steps, lower the energy needs and hazardous waste.
	Rational solvent selection, recycle and optimisation; reduction and avoidance of critical solvents
	Process intensification; novel equipment, and new processing methods
	Process Energy Intensity and Mass/Energy Integration; development of energy intensity metrics and refining mass and energy integration techniques within multioutput pharmaceutical plants
	Integration of chemistry and engineering; Chemistry and Chemical Engineering should operate seamlessly together if the desired outcome is an efficient, more sustainable process
LCA in pharmaceutical manufacturing	Generalized inclusion of life cycle thinking in product and process design and development and better understanding of life cycle inventory and impacts of pharmaceutical processes, bioprocesses, complex starting materials, and bioderived materials.
Reduce the environmental impact of pharmaceutical products	Improve degradability of pharmaceuticals; rational design of pharmaceutical compounds (benign by design) by Life Cycle Engineering
	Investigation and understanding of the behavior, fate and effects of drugs in the environment
	Support by the pharmaceutical industry in integrated and effective management of pharmaceutical waste
Supply Chain Integration	Integrated primary and secondary manufacturing to save transport costs, reduce inventories and avoid additional process steps and solvents

Source: Own compilation.

11 Nanotechnology

11.1 Summary

In the context of nanotechnology, the term “nanoscale” describes a size range from approximately 1 to 100 nanometres (nm)[44]. “Nano-objects” are discrete pieces of material with one, two or three external dimensions in the nanoscale. “Nanoparticles” are nano-objects with all external dimensions in the nanoscale, where the lengths of the longest and the shortest axes of the nano-object do not differ significantly. “Nano-plates” are nano-objects with one external dimension in the nanoscale and the other two external dimensions significantly larger. “Nanorods” are solid nanofibres, with nanofibres being defined as nano-object with two external dimensions in the nanoscale and the third dimension significantly larger. Nanomaterials are materials with any external dimension in the nanoscale or having internal structure or surface structure in the nanoscale. The dimensions of the particles or structures are typically between 1 and 100 nm.

For many years, the chemical industry has been producing many products using particles or structures with dimensions ranging from around 1 to 100 nm. They can be found e.g. in the form of irregular particles, spheres, platelets, fibres, tubes or layers. The optical, electrical and magnetic properties of nanomaterials, but also their hardness, toughness and melting behaviour are in some cases very different to those of conventional materials. Use of these nanomaterials has made it possible to create completely new products which are carefully customized to meet the specific requirements of a given application. Through addition of or coating with nano-objects, ceramics, metals and plastics can for example be developed which are scratch-resistant, nonreflective or water/grease/dirt repellent. Antibacterial surfaces or surfaces catalysing chemical reactions can also be made possible with nanomaterials.

Safe and sustainable usage of nanotechnology and nanomaterials in particular can offer many different and far-reaching approaches which will benefit mankind and the environment. Nanotechnology can therefore be one of the keys to solving the imminent problems faced by our society in a number of different pivotal areas of fundamental needs:

- the area of energy and mobility, where new materials can be used to achieve more efficient energy conversion on the basis of renewable energy sources and through improved, more efficient energy storage and usage.
- for protection of climate, environment and resources, among other things through more efficient usage of resources with the aid of specific catalysts and processes, and therefore also – e.g. thanks to the avoidance of unwanted by-products – the cleanup and rehabilitation of air, water and soil with the aid of nanomaterials.
- in terms of protecting and restoring health, for example through improved UV protection substances in sunscreens and textiles and through new treatment methods e.g. in the field of cancer treatments, but also in the area of packaging, which can help to increase the shelf life of food products in developing countries which would otherwise quickly go off on their way to the consumer.
- In the field of communication/information, microchips based on nano-scale switching elements are already an integral part of modern systems; these products have already been using “nanochips” for some time now. Storage media and new information processing concepts are surely set to continue this trend.

Consequently, major effort has been and is being put into research and development in order to turn the potential opportunities of nanotechnology into successful innovations. Nanotechnology is a field of intense research and innovation activities. Within the scope of this study, only an overview of different developments can be provided.

[44] ISO/TS 80004-1:2015(en) Nanotechnologies — Vocabulary — Part 1: Core terms

Some nanomaterials have already been well established in the marketplace for many years (e.g. carbon black in car tyres, titanium dioxide as UV blocker in sun cream or silver as anti-bacterial ingredient), others are in development or close to market entry. Some of these applications, such as the anti-bacterial nanoparticles for textiles can be debated as unnecessary and not beneficial from a sustainability point of view. Moreover, they can release material from the product to the technosphere and also to the ecosphere. It is necessary to debate the release of nanomaterials from product to the environment from the sustainable point of view.

Most nanomaterials applications aim at superior materials characteristics or improved customer benefits based on enhanced or additional functionalities. Nanomaterials may represent the major key for solving important challenges facing our society as outlined above. Nevertheless, the production, use and life-cycle impact of nanomaterials have to be carefully assessed case by case, to identify, which developments and applications are to be flagged as sustainable chemistry. The safety of nanomaterials including potential ecological and health implications of these materials, is subject to many research programmes.

In general, nanotechnology is a field of intense research activities and a wide variety of materials and applications are under investigation, sustainability needs to be assessed case by case. Table 18 provides an overview of the identified innovations in nanotechnology.

Table 18: Innovations in nanotechnology

Innovation approach	Example
Nanomaterials in electronics and optics	• Carbon nanotube as nanowires • Graphenes as optically transparent electrodes and substitution for indium tin oxide in solar cells and touch screen displays • OLEDs (Organic Light Emitting Diodes) with layer thicknesses in the region of nanometres for applications in colour displays
Nanomaterials for health	• Coated iron oxide nanoscale particles in magnetic resonance imaging as a medical contrast agent • Nanocarriers for drug delivery (e.g. protected against premature destruction , to improve uptake in the body, to provide selective release of the active ingredient, to overcome the blood brain barrier) • Coating of implantation materials with biocompatible or easy to clean surfaces complete with biocides or anti-adhesive properties
Nanomaterials for textiles	• High-tech textiles with improved breathability thanks to electrospun polymer nanofibres without any loss of protection against wind and rain • Water repellent nanoscale silicon dioxide for both self-cleaning and water-repellent fabric; despite these properties, the fabric remains able to breathe. • Nano coated textiles for antimicrobial coating
Nanomaterials for energy	• Carbon nanotubes in turbines of wind power stations for reduced weight and increased mechanical stability • Nanocomposites containing carbon nanotubes for super capacitors • Nanostructured electrode materials for lithium ion batteries • Nanoporous metal organic frameworks for the storage of hydrogen • Efficient catalysts for fuel cells • Fullerenes in organic photovoltaic modules

Innovation approach	Example
	• Quantum dots in Quantum dot photovoltaic modules
Nanomaterials in construction	• Nanocellulose for treatment of wood and hardboard • Titanium dioxide in facade paints or concrete surfaces, to reduce air pollutants like nitrogen oxides • Titanium dioxide in self-cleaning applications like on windows of high rise buildings • Hollow silica nanospheres for improved insulation effects on insulating materials for building construction
Nanomaterials for environmental applications	• Nano-structured titanium dioxide for photocatalytic water purification and removal of hazardous pollutants from wastewaters • Nanomaterials to replace (environmentally) toxic substances (i.e. flame retardants or toxic corrosion inhibitors) • Fe(0) for groundwater remidiation

Source: Own compilation.

The wide variety of materials and application fields require interdisciplinary and cross-sectorial research and development efforts for new innovations in nanomaterials. Collaborations of material scientists with the respective application sectors is mandatory, as well as environmental/sustainability experts. The huge field generally leaves ample room for innovative and fast acting small and medium-sized enterprises offering nanomaterials for specific applications or services. The nanowerk website provides a list of suppliers of nanomaterials.[45]

12 Research and Innovation funding

Funding programmes for research and innovation in the area of chemistry are manifold and specifically organized and structured in each country or region. Programmes exclusively dedicated to sustainable chemistry are an exception. A comprehensive global overview on chemistry programmes is beyond the scope of this document, subsequently, funding opportunities in Europe and the US are depicted as examples.

12.1 Europe

12.1.1.1 Horizon 2020

Horizon 2020 is the largest EU Research and Innovation programme with nearly €80 billion of funding available over 7 years (2014 to 2020). The programme follows the former EU Framework Programmes for Research (FP1-7) combined with the former Competitiveness and Innovation Programme (CIP), but has a stronger element of innovation funding, e.g. instruments such as pilot and demonstration activities or to bridge the gap between research and actual market deployment of research results. Funding opportunities under Horizon 2020 are set out in multiannual work programmes, which cover the large majority of support available. The work programmes are prepared by the European Commission within the framework provided by the Horizon 2020 legislation and through a strategic programming process integrating EU policy objectives in the priority setting.

[45] http://www.nanowerk.com/nanotechnology/nanomaterial/suppliers_a.php

The preparation of work programmes involves the consultation of stakeholders. For this purpose 19 Horizon 2020 Advisory Groups have been set up as consultative bodies representing the broad constituency of stakeholders ranging from industry and research to representatives of civil society. Additional open and targeted consultation activities aim to obtain further views and contributions, including from the Enterprise Policy Group[46] and European Technology Platforms.

Specific for sustainable chemistry two stakeholder initiatives should be mentioned explicitly:

- the European Technology Platform on Sustainable Chemistry – SusChem (www.suschem.org), operating since the preparation of FP7 and actively engaged in proposing and implementing topics on sustainable chemistry and biotechnology for FP7 and nowadays Horizon 2020 with huge success: a SusChem impact analysis calculated a total funding for SusChem relevant projects in FP7 of 1.4 Billion Euro, representing 6% of the total funding available for the FP7 Collaborative Research funding scheme.
- the Public Private Partnership “Sustainable Process Industry through Resource and Energy Efficiency” – SPIRE, which represents 8 process industry sectors, incl. the chemical sector as initiator and leading sector, steel, minerals, non-ferrous metals, cement, ceramics, engineering and water. This Public-Private Partnership with the European Commission as public partner was launched as part of Horizon2020 and regularly implements calls flagged as SPIRE calls in the work programmes of Horizon 2020.

The Horizon 2020 programme consists of three main research areas or "pillars":

- **Excellent Science** focuses on fundamental research. It includes instruments of the European Research Council (ERC) grants, funding for future and emerging technologies (FET) and researcher mobility (Marie Sklodowska-Curie Action) as well as large European research infrastructures.
- **Industrial Leadership** aims to speed up development of the technologies and innovations that will underpin tomorrow's businesses and help innovative European SMEs to grow into world-leading companies; it consists of three specific objectives:
  - "Leadership in enabling and industrial technologies" (LEIT) provides dedicated support for research, development and demonstration and, where appropriate, for standardisation and certification, on information and communications technology (ICT), nanotechnology, advanced materials, biotechnology, advanced manufacturing and processing and space.
  - "Access to risk finance" aims to overcome deficits in the availability of debt and equity finance for R&D and innovation-driven companies and projects at all stages of development.
  - grants“Innovation in SMEs" provides SME-tailored support to stimulate all forms of innovation in SMEs, targeting those with the potential to grow and internationalise across the single market and beyond.
- **Societal challenges** (SC) funds potential solutions to social and economic problems, funding focuses on the following challenges, several of them being relevant for the sustainable chemistry area:
  - Health, demographic change and wellbeing;
  - Food security, sustainable agriculture and forestry, marine and maritime and inland water research, and the Bioeconomy;
  - Secure, clean and efficient energy;
  - Smart, green and integrated transport;
  - Climate action, environment, resource efficiency and raw materials;
  - Europe in a changing world - inclusive, innovative and reflective societies;
  - Secure societies - protecting freedom and security of Europe and its citizens.

[46] http://ec.europa.eu/research/innovation-union/index_en.cfm?pg=eip"

In addition, the **European Research Council (ERC)** funding schemes are open to top researchers of any nationality or age who wish to carry out their frontier research in the 28 EU Member States or associated countries. There are three core funding schemes with eligibility based on experience of the applying researcher and his/her academic track record. One additional scheme is only for ERC grant holders.

Table 19: ERC grants

Type	Eligibility
ERC Starting Grants	researchers with 2-7 years of experience since completion of PhD; grants up to 1.5 million € for 5 years
ERC Consolidator Grants	researchers with 7 to 12 years of experience after PhD; grants up to 2 million € for 5 years
ERC Advanced Grants	Established researchers with recent track-record which identifies them as leader in their respective field of research; grants up to 2.5 million € for 5 years
ERCProof of Concept	For ERC grant holders, bridging gap between research and early stage of marketable innovation; grants up to 150,000 €

As the programme is thematically open and applications are bottom-up, there is no specific instrument dedicated to sustainable chemistry.

12.1.1.2 Research and innovation funding by EU member states

National research and innovation funding is different for each of the 28 member states. It is generally characterized by bottom-up fundamental research funded by organisations such as the German Research Foundation (DFG), the French National Research Agency (ANR) or the Netherlands Organisation for Scientific Research (NWO). Funding programmes for fundamental to applied research, innovation, pilot or demonstration activities is implemented through topical or open calls by different Governmental organisations nationally and regionally, but also by private or industrial foundations or organisations.

Table 20: Selected Funding Programmes of European Countries ERC grants

Country	Programme	Funding organisation	Character
Germany	FONA Research for Sustainability	Federal Ministry of Education and Research BMBF	Collaborative research
	From Material to Innovation		
	Environment Innovation Programme	Federal Ministry for the Environment	Industrial-scale pilot projects
France	Societal challenge 3 - Industrial renewal; Theme 4: Sustainable chemistry, products, related processes	French National Research Agency (ANR)	Collaborative research
Netherlands	Chemical Industrial Partnership Programme (CHIPP)	Netherlands Organisation for Scientific Research	Public-private co-operation

Country	Programme	Funding organisation	Character
UK	Funding competition: manufacturing and materials	Innovate UK	Collaborative research, at least 1 SME

Source: own compilation

12.2 US funding

12.2.1.1 Research funding by the NSF

The National Science Foundation supports a broad range of such chemistry research projects including sustainable chemistry, but the funding mechanism is essentially bottom-up and hence the NSF does not offer a specific programme for sustainable chemistry funding.

12.2.1.2 Green Chemistry Funding

EPA's Office of Research and Development, National Center for Environmental Research (NCER) funds research at academic institutions. Research in many areas of green chemistry may qualify for funding through Science to Achieve Results (STAR) research grants.

Fellowship funding for both undergraduate and graduate student environmental study that could be applied to green chemistry is also available.

Funding for small businesses is available under EPA's Small Business Innovative Research (SBIR) Program.

Many other government agencies offer SBIR funding for green chemistry technologies.

Funding is available for small businesses and research institutions working together under the Small Business Technology Transfer (STTR) Program.

12.2.1.3 Safer Chemicals Research Grants

EPA funds safer chemical research grants supporting the development of innovative science to support safer, more sustainable use of chemicals in consumer products and chemicals used for other purposes such as pesticides. Using safer, more sustainable chemicals will help to better protect human and environmental health, including sensitive populations like children, elderly and endangered species.

Recent Safer Chemicals Research Grants:

- Systems-Based Research for Evaluating Ecological Impacts of Manufactured Chemicals
- Organotypic Culture Models for Predictive Toxicology Center
- New Methods in 21st Century Exposure Science
- Susceptibility and Variability in Human Response to Chemical Exposure
- EPA/NSF Networks for Characterizing Chemical Life Cycle (NCCLCs)
- Development and Use of Adverse Outcome Pathways that Predict Adverse Developmental Neurotoxicity
- Developing High-Throughput Assays for Predictive Modeling of Reproductive and Developmental Toxicity Modulated Through the Endocrine System or Pertinent Pathways in Humans and Species Relevant to Ecological Risk Assessment
- Computational Toxicology: Biologically-Based Multi-Scale Modeling
- Increasing Scientific Data on the Fate, Transport and Behavior of Engineered Nanomaterials in Selected Environmental and Biological Matrices

- Environmental Behavior, Bioavailability and Effects of Manufactured Nanomaterials - Joint US – UK Research Program

More information and complete list under: https://www.epa.gov/research-grants/safer-chemicals-research-grants.

12.2.2 **Presidential Green Chemistry Challenge**

Federal government awards program of the EPA, has been recognizing innovative green chemistry research initiatives in business and academia since 1996. The Presidential Green Chemistry Challenge Awards promote the environmental and economic benefits of developing and using novel green chemistry. These prestigious annual awards recognize chemical technologies that incorporate the principles of green chemistry into chemical design, manufacture, and use.

EPA’s Office of Chemical Safety and Pollution Prevention sponsors the Presidential Green Chemistry Challenge Awards in partnership with the American Chemical Society Green Chemistry Institute® and other members of the chemical community including industry, trade associations, academic institutions, and other government agencies.
EPA usually presents one Presidential Green Chemistry Challenge Award in each award category. For the 2016 competition, there are six award categories:

- Focus Area 1: Greener Synthetic Pathways
- Focus Area 2: Greener Reaction Conditions
- Focus Area 3: The Design of Greener Chemicals
- Small Business (for a technology in any of the three focus areas developed by a small business)
- Academic (for a technology in any of the three focus areas developed by an academic researcher)
- Specific Environmental Benefit: Climate Change (for a technology in any of the three focus areas that reduces greenhouse gas emissions)

13 Regional Framework conditions: example Brazil

13.1 Summary

A survey by CNI, the National Confederation of Industry in Brazil, showed that 62% of the CEOs of innovative enterprises interviewed are of the opinion that the level of innovation in Brazil is low or very low and that industry prefers to import or copy innovations instead of creating them itself.

The National Pact for the Chemical Industry (2010) and the guidelines "Química Verde no Brasil (Green Chemistry in Brazil) 2010-2030" are possible drivers for Sustainable Chemistry. It is not clear, however, how binding these guidelines are.

One of the most important levers is the cost for energy and raw materials, where taxes and duties are also an important factor. In 2016, however, the government's cost-saving policy put a premature end to REIQ, the funding scheme with tax relief measures for the chemical industry for the purchase of specific raw materials.

Other (direct) cost factors are the costs for patenting or bureaucratic and legal requirements (product registration, planned introduction of GHS or a comparable system in the style of Canada's Chemical Management Plan (CMP)).

Other possible problems which come into question are lack of or limited access to finance, only weak links between science and industry, an often only low-skilled workforce and absence of or too complicated incentives.

On the other hand, there are various funding programmes and measures for research, development and innovation projects.

The Ministry of Science, Technology and Innovation supports innovations generated, amongst others, by accredited technology centres (Embrapii institutes).

Anprotec, the Brazilian Association of Science Parks and Business Incubators, fosters cooperation between Brazil and EU Member States in the areas of research, technology and innovation.

Apex-Brasil (Brazilian Trade and Investment Promotion Agency) offers special support for start-up enterprises.

With the exception of the biofuel sector, there are no relevant labels for sustainability criteria in the chemicals sector. This label could possibly be extended to other ethanol products: "Objectives: To develop a certification system that enables producers, buyers and others involved in sugar and ethanol businesses to obtain products derived from sugarcane that have been produced according to agreed, credible, transparent and measurable criteria." [47]

Table 21: Framework conditions for Sustainable Chemistry in Brazil

Country	Programme	Funding organisation
Incentives	Taxes	Taxes Tax advantages for renewable resources for the production of chemical raw materials in accordance with REIQ-Inovação (soon to expire).
	Co-finance	Innovation support /Accredited technology centres

[47] http://bonsucro.com/site/

Country	Programme	Funding organisation
		Similar to the Fraunhofer institutes, the Embrapii institutes funded by the Ministry of Science, Technology and Innovation are expected to raise a third of project funds amongst industrial customers.
	Funding	Funding schemes and measures Various funds and programmes with tax benefits and other support measures are available to enterprises for research, development and innovation projects.
Regulatory instruments	Chemicals management	Chemicals management The implementation of GHS (Globally Harmonized System of Classification and Labelling of Chemicals) is currently on the agenda in Brazil.
	Customs and duties	Customs and duties/ Free trade agreement NAFTA is proving to be an uncertainty.
Further framework conditions	Strategic planning	National Pact for the Chemical Industry, 2010 The National Pact for the Chemical Industry of 2010 shows "the investments needed in order to serve as outlines for the commitment of the chemical industry to the social and economic development of Brazil. It also identifies the greatest stumbling blocks to national and foreign investors' decision-making vis-à-vis expanding business in the Brazilian chemical sector. Removing these obstacles is an essential factor in the path that leads to the strengthening and the sustainability of the Brazilian economy."
	Guidelines	Guidelines: Química Verde no Brasil (Green Chemistry in Brazil) 2010 – 2030 A strategy to fully explore these comparative advantages is described in the text on: "Química Verde no Brasil (Green Chemistry in Brazil) 2010 – 2030" and is based on structuring a network of institutions, laboratories, pilot plants, and offices that are involved in research, development and innovation (R, D&I) on Green Chemistry.
	Links between science and industry	Anprotec – Brazilian Association of Science Parks and Business Incubators Anprotec, the Brazilian Association of Science Parks and Business Incubators (Associação Nacional de Entidades Promotoras de Empreendimentos Inovadores) founded in 1987, currently has about 300 members (incubators, science parks, educational and research institutions, government bodies) with about 400 business incubators and some 90 science park initiatives (Anprotec, 2016). There is no information about finance on the website; the statutes are only available in Portuguese. Anprotec is a partner in B.Bice, a European Commission project, which fosters cooperation between Brazil and

Country	Programme	Funding organisation
		EU Member States in the areas of research, technology and innovation.
	Support for start-up enterprises	Apex-Brasil (Brazilian Trade and Investment Promotion Agency) Apex-Brasil, the Brazilian Trade and Investment Promotion Agency, works to promote Brazilian products and services abroad and attract foreign investors for strategically important sectors of the Brazilian economy. It also takes care especially of the interests of start-up enterprises.
	Support for competing uses of national natural resources	National Programme for the Production and Use of Biodiesel (PNPB) The National Programme for the Production and Use of Biodiesel approved at the beginning of 2005 (Programa Nacional de Produção e Uso do Biodiesel – PNPB) is a targeted measure to foster the use of biodiesel in Brazil. In particular the production of biodiesel based on castor oil and palm oil is supported.
	Labelling	BONSUCRO — The Better Sugarcane Initiative In order to demonstrate compliance with the requirements of the EU, the third-largest customer worldwide for ethanol, with regard to the sustainability of the ethanol produced in Brazil, in 2011 the BONSUCRO certification system was introduced. The label could possibly also be extended to other ethanol products.

Source: Own compilation

14 Example of an assessment under consideration of sustainability aspects: Construction materials for thermal insulation

14.1 Question and approach

The question is raised which innovations can be subsumed under "sustainable chemistry". The approach selected here does not target the actual substance itself but instead how a substance or (raw) material is used in a particular application. "Thermal building insulation" was chosen as an example. Protection of buildings against high as well as low temperatures is playing an increasing role due to:

- Growing demands on air-conditioning in buildings
- The increasing number of buildings worldwide and the increase in living space per capita (documented for several industrialized countries and probable for other countries)
- Efforts to reduce energy consumption in buildings

Of course, energy consumption in buildings can be controlled to a considerable extent through user behaviour. In addition, the building's location, its direct surroundings, the design of the facade, the type of heating etc. play an important role. In this respect, numerous parameters which can lead to savings in the use of insulating materials need to be examined in order to find a holistic solution to the problem of "heating and ventilation in buildings". These alternatives are not discussed in the further course of the investigation, nor are aspects which result from poor ventilation (condensation, mildew, bad quality of indoor air etc.).

In order to classify innovative solutions in comparison to products long available on the market for insulating materials, a set of quantifiable indicators for sustainable chemistry [48] is used. These Parameters for Sustainable Chemistry (PSC) are usable above all for enterprises which produce chemical substances or use them in the manufacture of materials. Ideally, these are substance-related observations (hazardous content…) in conjunction with the respective production process (emissions, consumption of resources) and producer behaviour (supplier audits, investment intensity) as well as his success in the market.

The list of parameters drawn up on behalf of the German Environment Agency is presented in Table 22. and used as follows: In view of the data available from the cited publications and the depth of literature research which was possible, relative estimates are possible for the fields marked green. Whether the innovation results in an economic advantage can be assumed for those products and processes which have already been introduced into the market. In the case of the criteria marked violet, estimates are partially possible. The fields marked red are greatly dependent on the chosen production process, local conditions (e.g. availability of water) or the business philosophy of the specific enterprise and cannot be examined with regard to product properties.

The "other advantages" stated in the set of indicators refer here to the functionality of the material in its specific application.

Table 22: Set of indicators "Sustainable Chemistry Parameters" and their applicability for the topic in question

Indicator		
GHG emissions SDG F	Pollutant emissions into water	Economic advantages
Raw material use SDG B	Pollutant emissions into air	Certification in accordance with ISO, EMAS etc.
Percentage of raw materials made from renewables SDG B	Sustainability information on / about production	Investment intensity in environmental and / or resource protection
Raw material intensity / productivity SDG C	Waste generation SDG C	Staff training
Energy input	Percentage of hazardous waste	Total percentage of women
Energy intensity/ productivity	Hazardous substance content SDG A,D	Other advantages SDG E
Total water use SDG C	Occupational accidents SDG D	Market presence

[48] V. Abraham, M. Blepp, A. Joas, D. Bunke: Beiträge zur Nachhaltigkeitsstrategie – Minderung des Ressourcenverbrauchs in der Chemiebranche durch Instrumente der nachhaltigen Chemie, UFOPLAN *3713 93 425, Supplement to the 1st Interim Report, Berlin 2015; Umweltbundesamt, öko-Institut, Bipro: Set of indicators* "Sustainable Chemistry Parameters", March 2016

Indicator		
Percentage of recycled water SDG C	Occupational diseases SDG D	Monitoring of suppliers with regard to human rights and environmental aspects

Green fields: relative estimates are possible; violet fields: estimates are partially possible; red fields: indicator greatly dependent on chosen conditions

Some of the objectives from the SDGs have been interpreted in parallel by the authors with regard to the questions addressed here:

A) Benign by design chemicals: less risk to humans and nature (SDGs 3.9, 6.3, 12.4)

B) Functional chemicals from renewable materials and waste (SDGs 7.3, 12.2)

C) Providing far better yields, less waste, high-grade products (SDGs 7.3, 8.4, 12.5)

D) Enhancing occupational health (SDGs 3.9, 12.4)

E) New business models and more employment (SDGs 8.2, 9.5)

F) Higher energy efficiency and use of renewable sources (SDGs 7.2, 7.3)

They are partly compatible with the parameters listed above (Table 22). For conventional insulating materials including vacuum insulation panels (see below), the ÖKOBAUDAT[49] database also includes, in addition to figures on technical performance (here: insulating effect), information on energy consumption for production, GWP, ODP, volume of hazardous waste generated during disposal, water consumption etc. These data are for specific materials and originate from individual manufacturers. They only partly include information about additives. Where data was available it was also used for the comparative assessment.

14.2 Thermal building insulation - Principles

The ecological significance of thermal building insulation is reflected in the fact that in Europe far in excess of 50% of energy consumption connected to buildings is required for heating.[50] Its economic importance constitutes a market value in Western Europe alone of about € 6 billion.[51]

Rock wool and glass wool, together referred to as mineral wool, have been used for decades as a means of insulating buildings. They are produced from recycled glass as well as limestone, sand and soda or natural materials and sludge with added coke. They are either installed in the form of foam sheets with suitable binders or poured or blown in as loose material. Urea formaldehyde resins or phenol resins are mostly used as binders. The mineral substances exhibit a thermal conductivity of 30-40 mW/(m x K).

The second largest group (by market share in Europe) are organic polymers, above all expanded polystyrene (EPS) as well as the less often used extruded polystyrene (XPS) with a thermal conductivity of 30-40 mW/(m x K) and polyurethane (PUR) with 20-30 mW/(m x K).

In addition, insulating materials based on cellulose (amongst others treated recycled paper) and cork are used (both with 40-50 mW/(m x K)). All organic insulating materials must be treated with flame retardants. Fibre-based insulating materials must be sealed with a resin before use (phenol formaldehyde or urea formaldehyde resins). Due to health concerns with regard to formaldehyde, which is, however, for the most part sealed into the insulating material and should therefore release only traces of gas

[49] http://oekobaudat.de/datenbank/browser-oekobaudat.html, accessed on 27.7.2016

[50] European Commission, EU Energy, Transport and GHG Emissions, Trends to 2050 (Reference Scenario (2013).

[51] R. Benedix: Einführung in die Bauchemie für Bauingenieure und Architekten, 6th edition, Springer ISBN 978-3-658-04143-4 (2016), P. 547

(indoor air particularly strict regulations in France), binders based on sugar are meanwhile also being used ("ECOSE Technology", Knauf) as well as water-based acrylic binders (URSA). “However, to what extent the new sugar-based binder will prove itself in practice remains to be seen. Especially in cases where it is used for external building components such as roofs or facades, which pests such as insects and rodents like to infest, a sugar-based binder might be less likely to prevent infestation than an acrylic binder which to be sure does not offer insects, bacteria or mildew any breeding ground at all.”[52]

In view of the growing demand for energy-saving in buildings, developments are moving in the direction of a lower specific thermal conductivity, that is, thinner material with the same insulating effect. In the technical evaluation of materials for heat and cold protection, their acoustic properties, behaviour in case of fire and ease of installation play an important role. At conferences in the building sector a few years ago, targets for the further development of insulating materials were established, which can be found in Table 23[53] From the perspective of construction engineering there are, in addition to technical requirements with regard to specific properties in the areas of heat insulation, flame retardancy, insensitivity to damp etc., also requirements concerning the process of installing insulating materials, which have a major economic dimension.

Table 23: Requirements for future insulating materials (Jelle et al. 2010)

Property	Requirements
Thermal conductivity – pristine	<4 mW/(mK)
Thermal conductivity – after 100 years	<5 mW/(mK)
Thermal conductivity – after modest perforation	<4 mW/(mK)
Perforation vulnerability	Not to be influenced significantly
Possible to cut for adaption at building site	Yes
Mechanical strength (e.g. compression and tensile)	May vary
Fire protection	May vary, depends on other protection
Fume emission during fire	Any toxic gases to be identified
Climate aging durability	Resistant
Freezing/thawing cycles	Resistant
Water	Resistant
Dynamic thermal insulation	Desirable as an ultimate goal
Costs vs other thermal insulation materials	Competitive
Environmental impact (including energy and material use in production, emission of polluting agents and recycling issues)	Low negative impact

The area of building insulation is very nebulous, since apart from the actual insulating materials which are added to the masonry, supplementary solutions, such as insulating plaster or concrete with a low heat transition coefficient, are also available. There are also insulation boards on the market which are built up in layers composed of several different materials (sandwiches). For more than a decade now, what are known as heat-insulating bricks have also been available. These are filled with a wide variety of insulating materials, such as mineral wool, wood fibres or perlite, and exhibit thermal conductivity

[52] http://www.baulinks.de/webplugin/2010/1066.php4

[53] B.P. Jelle, A. Gustavsen, R. Baetens: The path to the high performance thermal building insulation materials and solutions of tomorrow, J. Build. Physics 34 (2), 99-123 (2010)

values of 70 – 80 mW/(m x K).[54] The sustainability aspects of the individual products can always only be assessed in conjunction with the respective building.

14.3 New materials for thermal insulation based on aerogels and vacuum technology

Since a few years, vacuum insulation panels (VIP) have been available on the market. “Vacuum insulation panels comprise a support core made of highly dispersed silica, infrared opacifier and cellulose fibres, which is sealed inside a metalized high-barrier foil under vacuum.“[55] In this way, a thermal conductivity of 4 mW/(m x K) is achieved which, however, more or less doubles in the course of about 10 years. Since it is necessary to drill into the sheets in order to attach them, this damage can produce values of up to 20 mW/(m x K). Vacuum panels are at present still far more expensive than conventional thermal insulation; since they cannot be cut to size in situ, they must be measured precisely before they are installed.

Aerogels, i.e. gels based on silica with very small pores (pore volume up to 90% of the material), achieve a thermal conductivity of about 13 mW/(m x K). The smaller and more finely distributed the pores are, the lower the thermal conductivity through the insulating material. However, the energy input needed to produce aerogels is considerable due to the high pressures and temperatures; they are made by extracting the water from silica.

Insulation boards with a gas filling in closed pores represent a further development in the area of aerogels. At nano scale, from pore diameters of about 10 nm thermal conductivity drops dramatically. Depending on the gas used, different insulating effects are achieved.[56] Figure 3 shows that the thermal conductivity in the case of air only falls short of the target value of 4 mW/(m x K), which VIPs also reach, at a pore diameter of about 50 nm, whilst the noble gases with increasing atomic weight even with larger pores with a diameter of up to 500 nm already exhibit such a low conductivity value. At a pore diameter of under 10 nm, thermal conductivity drops in the case of all the gases examined to almost 0.

[54] http://www.energie-experten.org/bauen-und-sanieren/daemmung/aussendaemmung/waermedaemmziegel.html, accessed on 7.8.2016

[55] http://www.oekobaudat.de/OEKOBAU.DAT/datasetdetail/process.xhtml?uuid=b4f9acf5-678f-4624-93e1-65515c8c3f86&stock=OBD_150820&lang=de, accessed on 28.7.2016.

[56] B.P. Jelle, A. Gustavsen, R. Baetens: Innovative High Performance Thermal Building Insulation Materials - Todays State-of-the-Art and Beyond Tomorrow. Lecture at Building Enclosure Science & Technology (BEST 3 - 2012), Atlanta, Georgia, U.S.A., 2-4 April, 2012.

Figure 3: Thermal conductivity of air and noble gases as a function of pore diameter

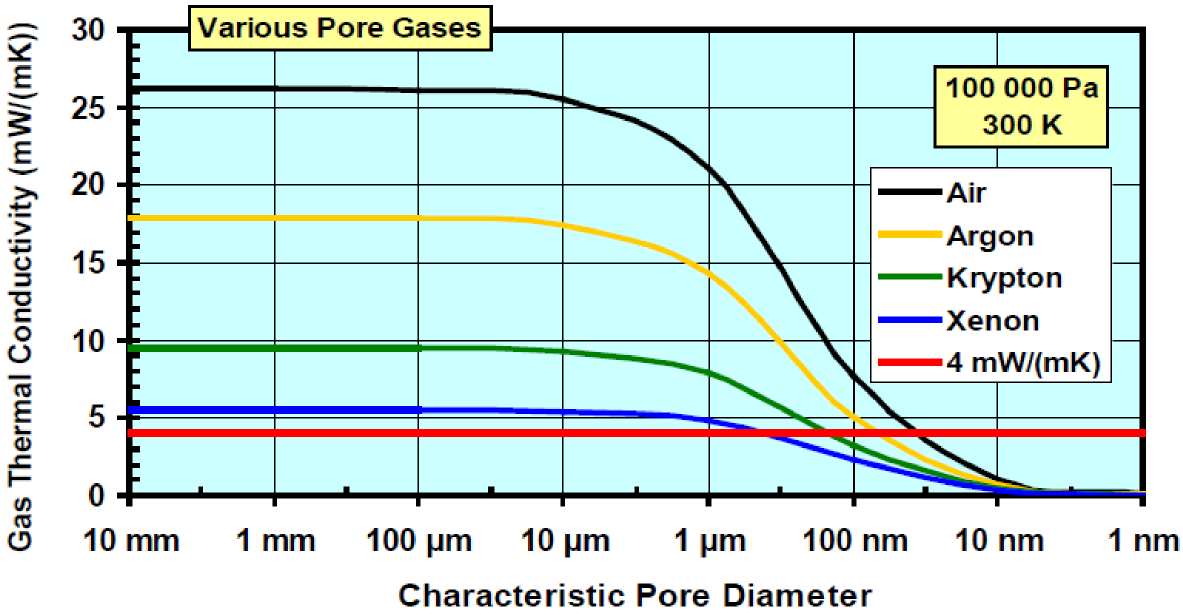


Table 24: Qualitative comparison of different insulating materials/insulating panels on the basis of same weight

	Cellulose fibre	Mineral wool (with glass)	Rock wool	PS EPS	PS XPS	PUR	VIPs	Aero-gels	Nano pores with gas
GHG emissions	0	+++	+++	++	+++	0	++	++	?
Energy input and energy intensity	+++	+	++	++	+++	+	+	+	?
Raw material input and percentage of renewable raw materials	Reproducible raw material and secondary raw material	Secondary raw material can be used		Made from crude oil	Made from crude oil	Made from crude oil	Silica, cellulose	Silica	Silica, noble gases
Waste generation In production… After use…	 + +++	 ++ +++	 +++ +++	 0 Recycling	 0 Recycling	 ? ++	 + +++	 ? +++	 ? +++
Raw material intensity		High	High	High	High	High			
Critical contents	FSM, binders	Phenol formaldehyde binder	Phenol formaldehyde binder	FSM	FSM	FSM			
Technical advantages/ disadvantages	Very thick layer, lined against damp	Good workability, thick layer	Good workability, thick layer	Good workability, thick layer	Good workability, thick layer	As insulating sheet with glass fibre or lined with aluminium	Only usable in panel form, thin layer	Good workability, thin layer	Good workability, thin layer

	Cellulose fibre	Mineral wool (with glass)	Rock wool	PS EPS	PS XPS	PUR	VIPs	Aero-gels	Nano pores with gas
Economic advantages [57], employment	Inexpensive	Inexpensive	Inexpensive	Inexpensive	Average price range	Average price range	High price range	High price range	?
Market presence	Average	High	High	High	Average	Average	?	?	No

57 Prices for insulating materials according to https://www.u-wert.net/10-daemmstoffe-im-vergleich/, accessed on 02.08.2016

14.4 Reducing cell size in polystyrene foam

Insulation boards made from polystyrene are composed of a foam wall which is relatively thick in comparison to the masonry itself. There is a great interest in obtaining thinner insulation boards above all for the external cladding of existing buildings in order to reduce refurbishment costs and avoid making a detrimental impact on the structure's aesthetic appearance. To separate polymers from the reaction vessel, what are known as nucleating agents are used, which should produce crystallisation nuclei which are as small as possible and thus also a homogeneous product. A new nucleating agent which entered the market a few years ago (Hydrocerol®, CaO on a LDPE carrier) makes it possible "to make a foam from light polystyrene with a significantly smaller cell size than that of foams currently available. Under the direct injection of gas, the newly developed formula[58] allows a reduction of the cell size from 200 to 50 µm in diameter. In addition, the optimized foam structure offers excellent insulating properties. The result is that manufacturers can produce strong and light insulation boards with improved insulating ability…"

Table 25: Qualitative comparison of polystyrene foams with cell sizes of about 200 µm and < 50 µm

Indicator	Polystyrene 200 µm	Polystyrene 50 µm
GHG emissions	+++	++
Energy input and energy intensity	++	+
Raw material input	Made from crude oil	Made from crude oil
Waste – Production Processing After use	0 +++ Recyclable	0 ++ Recyclable
Raw material intensity	High	Lower
Critical contents	Flame retardants (can hamper re-use)	Flame retardants (can hamper re-use)
Technical advantages/disadvantages	Thick layer	Layer about just half as thick
Economic advantages, employment, market presence	Inexpensive, commercially available	Presumably more expensive (Hydrocerol® supposedly on the market since 2015)

14.5 Infra-lightweight concrete

The construction sector is endeavouring to meet the increasing demands on thermal insulation with types of concrete which on the one hand display a lower heat transition coefficient and on the other hand are lighter than the concrete used to date yet without any reduction in load-bearing capacity (thus this is not an insulating material in the narrower sense). What is known as infra-lightweight concrete exhibits densities of under 800 kg/m^3. This is lower than that of conventional types of lightweight concrete where density ranges up to 2000 kg/m^3. The focus here is above all on a higher percentage of fine-

[58] http://newsroom.clariant.com/de/cmmd14_mr_masterbatches/

grain material in the concrete ("Microsilica"), which results in a higher packing density in the fine material and a higher percentage of pozzolans. "Infra-lightweight concrete as load-bearing thermal insulation permits a broad range of applications in the area of monolithic exposed concrete structures and, due to its low weight, for large prefabricated elements too. In this way, wall structures which are difficult to produce, susceptible to faults when being installed, problematic in terms of maintenance and disposal can be circumvented. Infra-lightweight concrete promises inexpensive, permanent and easily recyclable exposed concrete structures."[59] With the aggregates named above, a far lower energy input is required for cement production; such composite cements contain <50% Portland cement clinker.

Table 26: Qualitative comparison of conventional types of concrete and heat-insulating concrete

	Concrete (made exclusively from Portland cement)	**Lightweight concrete**	**Infra-lightweight concrete**
GHG emissions	+++	++	+
Energy input and energy intensity (production)	+++	++	+
Raw material input	Widely available mineral raw materials	Widely available mineral raw materials	Widely available mineral raw materials
Waste generation Processing After use…	 0 Re-utilisation possible	 0 Re-utilisation possible	 0 Re-utilisation possible
Raw material intensity	High	A little lower	Lower
Critical contents	Depending on the origin, e.g. Cr VI, heavy metals from the use of waste as energy source	Depending on the origin, e.g. Cr VI, heavy metals from the use of waste as energy source	Depending on the origin, e.g. Cr VI, heavy metals from the use of waste as energy source
Technical advantages/ disadvantages	High weight influencing other parts of the construction	Lower weight	Lower weight; thermal insulation effect
Economic advantages, employment	Cheap production, well-known technology		Lowers need for additional thermal insulation
Market presence	High (presumably decreasing)	Presumably increasing	Presumably increasing

14.6 Insulating foams made from fungal mycelium

Fungal mycelia, which grow on agricultural waste, are already being used in packaging manufacture. A US-American firm is working on the development of other fields of application for fungal mycelia, including interior construction (binders for chipboard panels, insulating foams). "We bind particles together with our natural resin. We make molded shapes or large panels, and also thin ply materials that are more flexible… Replace plastic foams like Styrofoam with our Earth friendly alternative!" According

[59] M. Schlaich, K. Hückler: Infraleichtbeton 2.0. Beton- und Stahlbetonbau 107 (11), 757–766 (2012)

to the company, the development of its insulating material is currently being supported by the EPA.[60] The material does not seem to be commercially available yet. The permanent technical functionality when using organic materials which are in principle compostable is undoubtedly a challenge.

Table 27: Qualitative comparison between insulating materials made of fungal mycelium and polystyrene

Indicator	Polystyrene	Fungal mycelium
GHG emissions	+++	Presumably low
Energy input and energy intensity	++	0
Raw material input and percentage of renewable raw materials	Made from crude oil	Renewable raw material
Waste – Production	0	?
Processing	+++	?
After use	Recyclable	Presumably not re-usable
Raw material intensity	High	?
Critical contents	Flame retardants (can hamper re-use)	Flame retardants Possible hazard from fungal spores during production
Technical advantages/ disadvantages	Thick layer	No information
Economic advantages, employment	Inexpensive	Fungi cultivation likely to be more labour-intensive than production of PS
Market presence	High	Development and pilot phase

14.7 Composite insulating panels

Insulating boards made of a very wide variety of different materials are marketed under the name of “sandwich panels”, e.g. PUR rigid foam with an aluminium shell (Alutherm®), rock wool with a steel shell (Paroc) or concrete with a layer of insulating material inside. By contrast to insulating materials, they do not require any weather protection, i.e. plaster or masonry.

The precast concrete sandwich panel[61] is composed of a facing layer as a visual design element and a base layer. Between the two there is a layer of air and a layer of thermal insulation, e.g. XPS, EPS, PUR rigid foam or fibre-based insulating material. Recycled concrete is today not only used in civil engineering but also as an additive to new concrete in building construction. The use of recycled concrete can

[60] According to the firm’s website, http://www.ecovativedesign.com/materials, accessed on 24.04.2016

[61] St. Heeß: Mehr als nur Fassade, http://www.dyckerhoff.com/online/download.jsp?idDocument=177&instance=1, accessed on 02.08.2016

reduce the cost for the production of composite building components above all in locations where there are no cement factories and the raw material can be recovered from demolition material. Over 50% of what is known as the ECO-SANDWICH® comprises secondary raw material. Figure 4 shows the structure of such a building component: On the side facing the interior of the building there is a 12 cm thick layer of recycled concrete, then 20 cm of mineral wool, followed by a layer for ventilation purposes which is 4 cm thick and an external skin 6 cm thick where crushed bricks from demolition material are used.[62] A comparison to a precast concrete panel used for a hotel and administrative building is shown in Table 28, whereby no details are available on this product's structure.

Figure 4: ECO-SANDWICH®

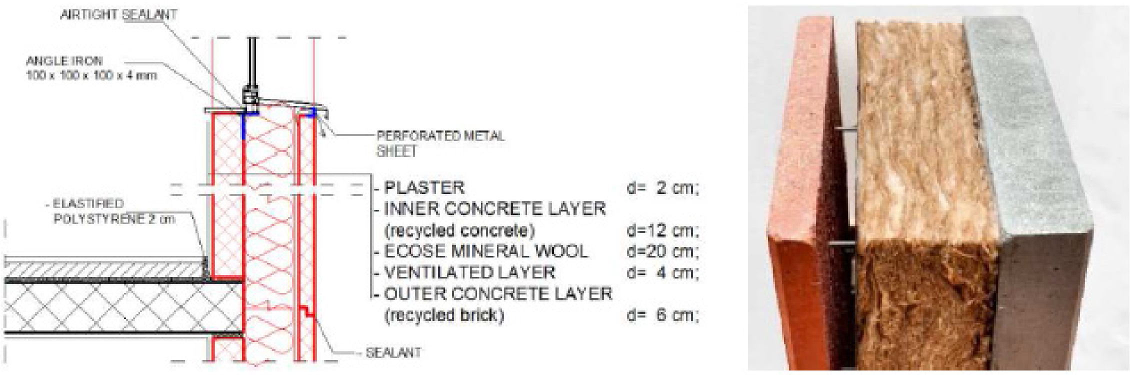


Table 28: Qualitative comparison of a conventional precast concrete sandwich board and the ECO-SANDWICH®

Indicator	Precast concrete sandwich board	ECO-SANDWICH®
GHG emissions	+++	+
Energy input and intensity	++	+
Raw material input	Widely available mineral raw materials	Partly mineral secondary raw materials
Waste – Production	0	?
Processing	+	+
After use	Recyclability questionable	Presumably not recyclable
Raw material intensity	High	Average
Critical contents		Possibly phenol formaldehyde resins
Technical advantages/ disadvantages	Prefabricated element for the facades of large buildings	Presumably also intended for residential buildings

[62] M. Alagusic, B. Milovanovic, I. Banjad Pecur: Recycled aggregate concrete – sustainable use of construction and demolition waste and reduction of energy consumption. Advances in Cement and Concrete Technology in Africa Proceedings 2nd International Conference (Eds.: W. Schmidt, N.S. Msinjili), 253-262, Berlin 2016 (ISBN: 978-3-9817502-3-2)

Indicator	Precast concrete sandwich board	ECO-SANDWICH®
Economic advantages, employment	Inexpensive, easy workability	Labour-intensive due to complex manufacture; presumably competitive in low-wage countries
Market presence	High	Not known

In a publication which appeared recently, the insulating effect of different composite materials are examined together with the respective ecological aspects. In the LCA, the most efficient insulating materials (i.e. those with a particularly low heat transition coefficient) often score worse because they contain substances such as epoxy resins.[63]

14.8 Insulating materials made from renewable raw materials

Having evaluated available literature sources, it can be said that plant raw materials such as jute, hemp and flax are already being used on a small scale to produce insulating material. Their areas of application are limited. For example, perimeter insulation (outside insulation where building components are in direct contact with the ground) is not possible with hemp.[64] The fibre fleece may, however, contain support fibres made from polyester in a ratio of about 15%.[65] Ammonium phosphate or ammonium sulphate, for example, is used as flame retardant. The objective of the development as described in literature is to produce insulating materials from renewable raw materials which display comparable physical and mechanical properties to those of conventional materials. An additional advantage lies in the fact that natural building materials can regulate humidity in indoor spaces better. However, the decreasing effect of heat insulation as the water content of the material increases must be taken into account.[66]

A comparative overview of numerous "unconventional" insulating materials (renewable raw materials and waste) arrives at the conclusion that some such materials measure up well in comparison to polymers such as EPS with regard to insulating properties as well as acoustics and in some cases also score better. Overall, however, many questions are still unanswered: "In conclusion there are still issues that remain to be solved before a widespread use of unconventional materials. Some properties should be further investigated such as durability, fire resistance, water vapour diffusion, fungal resistance in particular for the best performing materials. An important requirement influencing the sustainability of these insulators is related to the availability of its components since the use of local materials lead to a reduction of economic and environmental impacts. The production of insulators made of natural materials should not be in conflict with the plantation and harvesting of food crops, but it should be focused on using residues and by-products of the agricultural sector."[67] The expectations placed in the early

[63] A.D. La Rosa, A. Recca, A. Gagliano, J. Summerscales, A. Latteri, G. Cozzo, G. Cicala: Environmental impacts and thermal insulation performance of innovative composite solutions for building applications. Construction and Building Materials 55, 406–414 (2014)

[64] http://www.energieheld.de/daemmung/daemmstoffe/hanf, accessed on 7.8.2016

[65] See, for example, datasheet for hemp fleece at ÖKOBAUDAT: http://www.oekobaudat.de/OEKOBAU.DAT/datasetdetail/process.xhtml?uuid=5ef0c519-f5b2-4d45-809d-5f417f90e90b&stock=OBD_150820&lang=de, accessed on 02.08.2016

[66] A. Korjenic, V. Petránek, J. Zach, J. Hroudová: Development and performance evaluation of natural thermal-insulation materials composed of renewable resources. Energy and Buildings 43 (9), 2518–2523 (2011)

[67] F. Asdrubali, F. D'Alessandro, S. Schiavoni: A review of unconventional sustainable building insulation materials. Sustainable Materials and Technologies 4/2015, 1-17 (2015)

years on the long-term stability of such materials against attacks by mildew[68] have evidently – at least not in general – not been fulfilled.

14.9 Energy storage with phase change walls

Latent energy storage systems based on materials which absorb energy during the change between solid and liquid phase and give off corresponding specific crystallisation energy upon cooling have been known for a long time. Due to the very short transport routes, their application in walls is interesting because the temperature differences are small. A substantial number of buildings with such installations meanwhile exist. "The integration of phase change materials (PCM) in building walls is a way to enhance the storage capacity of building envelope and then to rationalize the use of renewable and non-renewable energies."[69] Both inorganic salts with large hydrate shells are used as well as paraffins. To a lesser extent eutectic mixes are evidently also used. In 2015, global sales of such systems reached about US $ 1.5 billion with annual growth rates of about 30%. Their interaction with solar thermal systems is likely to contribute to a considerable reduction of energy input in residential and commercial buildings.[70] The phase change materials are installed, for example, in special bricks or inserted as an intermediate layer in sandwich panels. Applications in the form of microcapsules seem to be playing an increasing role. **"**Microencapsulation is one of the well-known and advanced technologies for better utilisation of PCMs with building parts, such as, wall, roof and floor besides, within the building materials. Phase change materials based microencapsulation for latent heat thermal storage (LHTS) systems for building application offers a challenging option to be employed as effective thermal energy storage and a retrieval device."[71] BASF manufactures such a system under the name of Micronal® PCM, where the capsules are about 5 µm in diameter.[72] The material can be used in corresponding sandwich panels made, for example, from gypsum, which in turn are marketed as products for the construction sector by manufacturers such as Saint Gobain.

Whilst the advantages for the energy consumption of the building in operation are obvious, the use of phase change building components needs also to be considered from the perspectives of building demolition, energy input for production as well as raw materials required in order to gain an idea of the sustainability of such solutions.

14.10 Focus of innovations

Which innovations can be subsumed under "sustainable chemistry"? In contrary to the usual rules for green chemistry, it is not sufficient to focus on the chemicals itself and their production processes. With respect to the other dimensions of sustainability in general and to important interfaces with resource management (recycling after use, longevity of the product…), energy efficiency and climate effects in the use-phase among others, it was decided to examine a group of materials in a distinct field of application. As sustainability strategies include efficiency, consistency, and sufficiency, application fields related to a well-defined area of need seem to be a good gateway to sustainability assessments. Thermal insulation

[68] W. Hofbauer, T. Rennebarth, K. Breuer, K. Sedlbauer: Die dritte industrielle Revolution am Bau auf biogener und bionischer Basis. Chemie Ingenieur Technik 81 (11), 1733-1742 (2009)

[69] F. Kuznik, D. David, K. Johannes, J. Roux: A review on phase change materials integrated in building walls, Renewable and Sustainable Energy Reviews 15 (1), 379–391 (2011)

[70] N. Soares, J.J. Costa, A.R. Gaspar, P. Santos: Review of passive PCM latent heat thermal energy storage systems towards buildings' energy efficiency, Energy and Buildings 59, 82–103 (2013)

[71] V.V. Tyagi, S.C. Kaushik, S.K. Tyagi. T. Akiyama: Development of phase change materials based microencapsulated technology for buildings: A review, Renewable and Sustainable Energy Reviews 15, (2), 1373–1391 (2011)
[72] http://www.micronal.de/portal/basf/ien/dt.jsp?setCursor=1_290868, accessed on 15.04.2016

of buildings offers an interesting field for this approach because of the high number of connections and interfaces with resource management, energy consumption, preventive fire protection, interior climate, new business models and other subjects. In this case, "habitation" is the area of need. Thermal insulation has to be optimised with respect to the efficiency of space heating. We used the information collected on innovative materials for building isolation as compared to materials which have already been long on the market (chapter 9).

In order to classify sustainable innovations, two approaches were used: The Parameters for Sustainable Chemistry (PSC) which have been developed for enterprises which produce chemical substances or use them in the manufacture of materials. Part of these parameters can be applied for the assessment in question. For the other approach, Sustainable Development Goals being of relevance for sustainable chemistry were selected. The focus on applications comprising very different solutions provided by combinations of techniques with varying chemicals and materials allows a comparison of all methods for building isolation. Especially with respect to the selected SDG's, numerous contributions to sustainable development can be found. On the other hand, conflicting goals can be detected which make trade-offs necessary if no better alternatives fulfilling more goals without conflicts are available. As to the Parameters for Sustainable Chemistry, also semi-quantitative assessments are possible depending on the availability of reliable data. But this set of parameters should be reviewed and restructured adding evaluation criteria which are relevant for applications. The difficulties showing up for a proper assessment can be demonstrated by the enormous variety of complete or partial solutions in this case study, since apart from the actual insulating materials which are added to the masonry, supplementary solutions, such as insulating plaster or concrete with a low heat transition coefficient, are also available as well as sandwich insulation boards, heat-insulating bricks and - in near future – nanoporous material filled with noble gases.

Obviously, "sustainable products" are not in the focus of the producers, but products with an added-value for more sustainable solutions as compared to existing products. Moreover, "sustainable solutions" can always only be assessed in conjunction with the respective building in its surroundings due to dependencies of the local conditions, e.g. climate, available natural resources. This leads to the conclusion that indicators or yardsticks for the SDGs in question should be available in future to be used mindfully with respect to potential conflicting goals.

The innovations summarized in Table 29 show different ecological goals and refer to various stages in the life cycle. This underlines the difficulty in assessing materials in the context of sustainable chemistry. Generally speaking, there are incremental approaches, i.e. no developments which are holistic or at least address several aspects.

Table 29: Goals targeted by the innovations under consideration

Innovation	Life cycle	Goals
Thinner insulating panels from polystyrene by producing smaller pores **D→M**	Manufacturing, construction and use phase	Reduction of resource consumption; improvement of construction
New insulating materials based on nano pores on the basis of silica **M**, filling with noble gases **D**	Choice of raw material and use phase	Reduction of energy for heating/cooling, use of a simple raw material
Insulating foams made from fungal mycelium **R**	Choice of raw material	Use of renewable raw material, decrease of energy demand for production

Innovation	Life cycle	Goals
Composite panels for insulation purposes using renewable raw materials ("ECO Sandwich") **D→M**	Choice of raw material	Restriction to cheap materials, use of demolition waste
Insulating materials based on renewable raw materials (plant fibres) **D→M**	Choice of raw material	Based on plant fibres, partially from residues and by-products
Infra-lightweight concrete (< 800 kg/m³) with high percentage of fine-grain materials – "Microsilica" **D→M**	Production phase, construction of buildings	Decreasing energy consumption and GHG emissions; technical prerequisite for reduction of insulation material

R = Research; D = Development; M = Available on the market

Source: Own compilation

14.11 Addendum

The "Guideline for Sustainable Building" (Leitfaden Nachhaltiges Bauen)[73] can be helpful when assessing building materials in their areas of application. In the case of more thorough analysis, it should be examined with regard to its applicability. The guideline published by the Federal Ministry for the Environment, Nature Conservation, Building and Nuclear Safety is intended above all for the planning of new buildings or refurbishment work with a holistic approach to the building over its whole life cycle.

DIN EN 15643 defines sustainability requirements for buildings and structures, whereby the economic, socio-cultural and ecological aspects are supplemented by technical and functional requirements (this is a further dimension in the "Guideline for Sustainable Building") as well as process quality of planning and execution (P. 17 of the guideline). The sustainability assessment includes the life cycle of the building from planning to construction, use, maintenance, refurbishment, demolition, re-utilisation and disposal.

15 Example of an assessment under consideration of sustainability aspects: Comparison of production routes for acrylic acid

15.1 Question and approach

Contrary to chapter 14, the focus of this assessment example is the investigation of different production routes for a given target product, thereby using a variety of feedstock. As in the case of the previous example, the "Sustainable Chemistry Parameters"[74] will be used. The chosen target product is acrylic acid, the principle building block for sodium acrylate, an important base material for high-performance polymers which are used for example as super absorbers in baby diapers. Annual worldwide production exceeds 3 million tonnes.

[73] Bundesministerium für Umwelt, Naturschutz, Bau und Reaktorsicherheit: Leitfaden Nachhaltiges Bauen, Berlin 2016. http://www.nachhaltigesbauen.de/fileadmin/pdf/Leitfaden_2015/LFNB_D_final-barrierefrei.pdf, accessed on 27.7.2016.

[74] V. Abraham, M. Blepp, A. Joas, D. Bunke: Beiträge zur Nachhaltigkeitsstrategie – Minderung des Ressourcenverbrauchs in der Chemiebranche durch Instrumente der nachhaltigen Chemie, UFOPLAN *3713 93 425, Supplement to the 1st Interim Report, Berlin 2015; Umweltbundesamt, öko-Institut, Bipro: Set of indicators* "Sustainable Chemistry Parameters", March 2016

15.2 Fossil-based acrylic acid production

The established current production route for acrylic acid, used as reference for the comparison is the partial oxidation of propylene, which itself mainly originates from steam cracking of Naphtha. The process involves two reactors, utilizing two separate catalyst systems. The first reactor converts the propylene to acrolein while the second reactor completes the conversion from acrolein to acrylic acid. The resulting acrylic acid is 100% fossil based. Table 30 shows some relevant process parameters.

Table 30: Cost and carbon footprint of propylene route to acrylic acid[75]

	Consumption unit/kg	Variable cost €/kg product	Carbon footprint kg CO_2/kg
Average		0,81	0,74
Steam		0,00	0
Electricity	1,22	0,03	01769
Fuel	0,23	0,00	0,0166
Propylene	0,854	0,74	0,5493

15.3 Acrylic acid from renewable feedstock

A number of alternative routes to acrylic acid using renewable feedstock can be considered. As byproduct of biodiesel production, glycerol is an interesting feedstock. Synthesis of propylene from glycerol is possible, the route consists of the formation of 1-propanol as intermediate through hydrogenolysis of glycerol at a high selectivity followed by subsequent dehydration to propylene. Via this route, acrylic acid production can partially or fully be based on renewable feedstock. Alternatively, acrylic acid can be directly produced from bio-derived glycerol by selective dehydration to acrolein and subsequent oxidation or in a one-step oxydehydration.[76]

Another route is the fermentation of carbohydrates to 3-hydroxyproponic acid followed by dehydration.[77] Finally, acrylic acid can be synthesized from CO_2 and ethylene, the latter can be bio-based from ethanol. Table 31 provides a qualitative assessment for the different sustainability indicators.

Table 31: Sustainability impact of different routes to acrylic acid

	Propylene	Renewable propylene	Glycerol	Sugar (fermentation	CO_2 and bio-ethylene
GHG emissions[78]	0,74 kg/kg	-1,76 kg/kg	1,43 kg/kg	-3,15 kg/kg	-0,6- -1,8 kg/kg [79]
Energy input and energy intensity	o	++	++	++	+++ bio-ethanol synthesis

75 Numbers from SRI Process Economic Reports
76 ARKEMA patent WO 2006/114506
77 Dow Chemical Company and OPXBio, https://pubs.acs.org/cen/news/89/i16/8916notw5.html
78 From: DSM: Route Scouting guided by modeling "Winning Key Renewable Raw Materials
79 Project ACER, BASF

Raw material input and percentage of renewable raw materials	o 0%	++ 0-100%	+ 100%	+ 100%	+ 0-100%
Waste – Production					
Raw material intensity	o	+ land use	+	+ Potential food compeition	+
Critical contents	o	o	o	o	o
Technical advantages/ disadvantages			Coupled to biodiesel production		Distillation of ethanol from water
Economic advantages, employment		High feedstock cost	Side stream valorisation	High feedstock cost	High feedstock cost
Market presence	98%	Low	low	low	Low
Total water use	o	++ Agriculture	++ agriculture	++ agriculture	++ agriculture

15.4 Conclusions

For evaluating of the sustainability of different production pathways and feedstock, it is mandatory to carefully assess all sustainability indicators. Generally the biomass routes are advantageous in terms of GHG emissions but effects are often lower than usually expected, if a cradle to gate analysis is made and all effects including crop cultivation, fertilizers, harvesting, transport, land use etc. are taken into account. Sucrose and starch biomass have the additional critical aspect of potential food and feed competition, an aspect that gains impact if one of these routes evolve into commercial operation on large scale. Lignocellulosic biomass such as wood (in particular waste wood), or waste biomass are of course less critical in this respect. Aspects such as water footprint and land use have also to be considered for the biomass routes. In addition, biomass routes are also characterised by a substantially higher energy demand, as the process efficiency is lower and additional effort in feed preparation and product isolation and purification are necessary. In these categories, the sugar-based biomass is usually superior to lignocellulosic biomass, which needs additional pretreatment steps. Biomass utilisation efficiency is also to be considered. This can be very low, i.e. several tons of biomass are required to produce a ton of product. This is usually the case for the production of bio-based petrochemicals such as ethylene and propylene, which are listed in Table 31 as reactants. Usually it is more atom-efficient to directly target products with chemical functions including hydroxyl groups, carboxylic groups etc., rather than the basic building blocks of petrochemistry, for which the biomass feedstock has to be deprived of all oxygen, only to re-introduce oxygen-containing chemical groups in subsequent reaction steps. In this sense it is also advised not only to perform a cradle to gate LCA for one given route, but to also compare different utilisation routes for a given feedstock to identify the best options. This is particularly recommended for feedstock of limited availability, such as biomass.