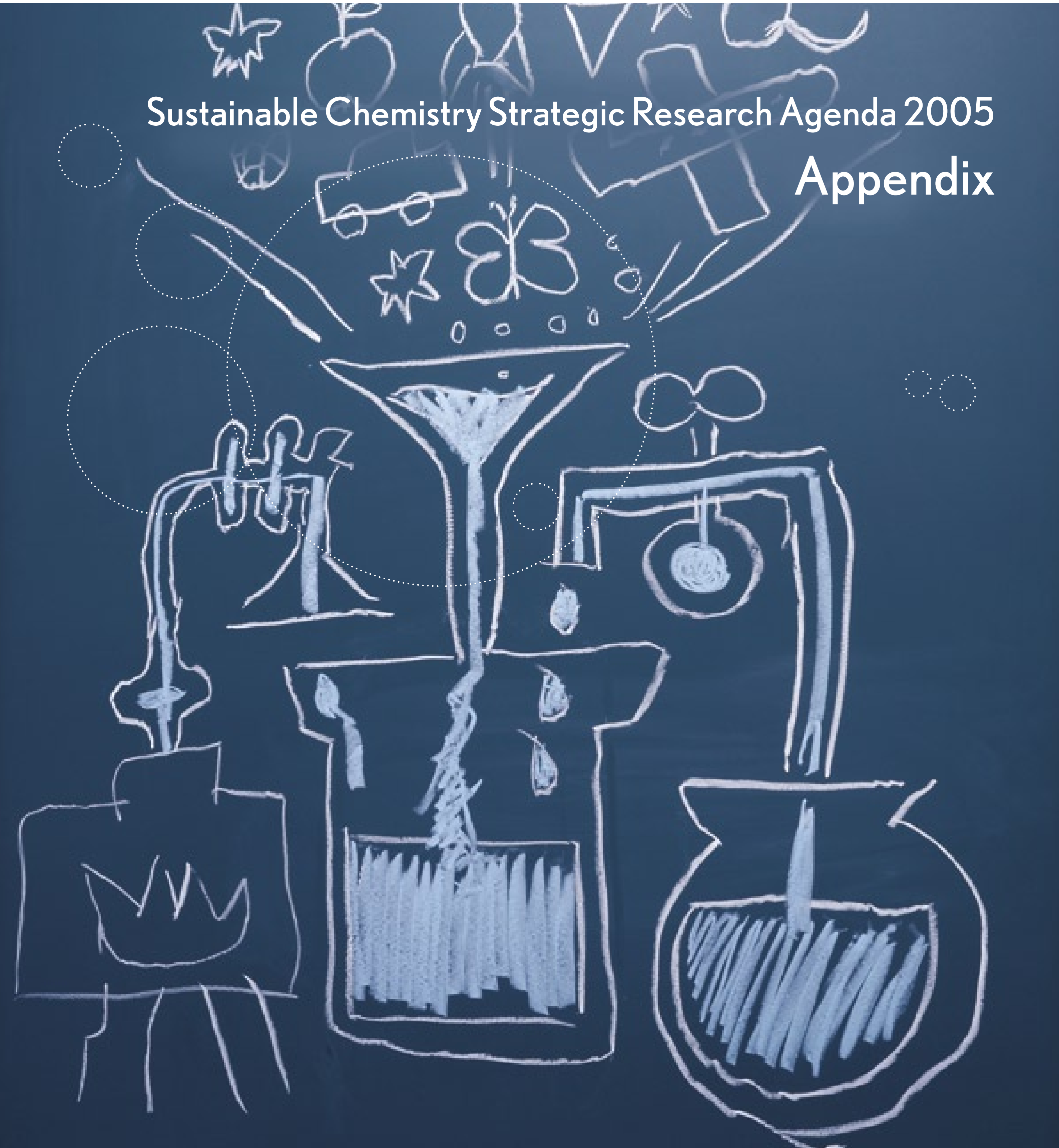
SusChem
European Technology Platform For
SUSTAINABLE CHEMISTRY

# Innovating for a Better Future



# Sustainable Chemistry Strategic Research Agenda 2005

## Appendix

# Contents

# Introduction

The Strategic Research Agenda outlines a strategy to achieve the SusChem vision. It identifies strategically important issues with high societal relevance in the areas of chemistry and industrial biotechnology; determines the challenges in these areas; and defines R&D priorities, timeframes and budgets. Achieving Europe's future growth, competitiveness and sustainable development objectives is, in the medium to long-term, dependent upon major research and technological advances in the areas defined by this Strategic Research Agenda. The SusChem research agenda offers a unique opportunity to focus European spending in chemical R&D on the most promising areas with respect to their impact on these overall goals.

The Strategic Research Agenda has been developed by three individual technology working groups looking at Materials Technology, Reaction and Process Design, and Industrial Biotechnology, and by a fourth working group concentrating on Horizontal Issues. Additional contributions have been received from an Industry Steering Group, and a Member States Mirror Group representing the national research authorities.

The intention of this Appendix is to provide the reader of the Strategic Research Agenda (SRA) with a more detailed discussion of the topics and themes highlighted by the SusChem working groups in the main document. The first section of the appendix deals with the product and technology roadmaps for energy (presented as example in the chapter *People, Planet, Profit* of the SRA); information and communication technology; healthcare; quality of life; citizen protection; and transportation. Through prioritisation (medium, high and essential) over short-, medium- and long-term timeframes, these roadmaps illustrate the selected products and technologies that should be pursued. This is followed by detailed discussions of the contributions to the SRA from the Industrial Biotechnology, Materials Technology, Reaction and Process Design, and Horizontal Issues working groups. The document concludes with the list of contributors.

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# Product and Technology Roadmaps

*To provide a coherent picture of (potential) development priorities, roadmaps illustrating products and technology developments for energy, information and communication technology, healthcare, quality of life, citizen protection and transportation have been created. These roadmaps provide guidelines and set the priorities (medium, high and essential) over the given timeframes (short, medium, long term) for research topics. For each product a list has been made with the current development status, the current or potential market volume and potential market success of that product. Associated with each product roadmap is a technology roadmap, indicating which technology developments are required to achieve and realise the products listed.*

*Since new results and insights influencing these roadmaps are gained basically every day, SusChem aims at updating its roadmaps on a regular basis.*

## 1 Products and Technologies for Energy Management

Whether in the form of electricity, heat, light, mechanical, biological or chemical, energy will become an ever more expensive commodity, and therefore there is a great need to manage this resource effectively. New products made from new advanced materials can have a large impact by providing better storage, consumption or transportation of energy. For the implementation of advanced materials in existing or new systems, interdisciplinary scientific research between organic and inorganic chemistry and material technology is vital. Beyond this, collaboration with process design engineers and biotechnologists is imperative.

### Alternative energy sources

Alternative sources of energy such as solar cells, fuel cells and renewable primary products are currently being investigated. These alternatives have great potential to find real life applications within the next ten years. The degree of success and implementation of the energy generation technologies mentioned above depends on developments in material science, which will overcome the current limitations of performance, stability and costs. If solar cells are to provide an alternative to fossil fuels, significant research needs to be done to develop new routes of crystalline silicon production in the development of amorphous silicon hybrid materials. This could result in enhanced efficiencies, concerted efforts for cheaper and more stable dyes, and improvement of the efficiency of the dye sensitised cells. The development of the fuel cell, from prototype via small-scale production to a mass product, can only happen if significant improvements are made to individual key components, and the corresponding contributions from the world of chemistry are absolutely vital. Material science needs to provide new proton exchange membranes that work at higher temperatures and new ecological catalysts for the reforming reaction. Other avenues being pursued are the generation of fuels from renewable bio-mass sources (especially lignocelluloses sources) to yield products like syngas, bioethanol or biodiesel. Advanced products will play a crucial role in making energy producing processes such as biorefineries eco-efficient and economically viable, providing an edge over other (fossil fuel) energy production processes.

## Energy management

New materials with useful conducting and superconducting properties will have a significant impact on our society in practical systems for the transmission of large electrical currents over long distances without energy losses. New types of longer-lasting rechargeable batteries as well as supercapacitors able to store more energy per volume and per weight are required for mobility (cell phones, laptops, etc.) and for increasing the efficiency of the hybrid engines used for physical transport. The development of new lower cost ceramic and metal composites with new mechanical properties will play a very important role in the creation of complex systems for a range of applications in the fields of energy creation and transport.

The fuel consumption of cars will be reduced by substituting steel with lighter polymeric materials in automobile construction, and by increasing the efficiency of petrol and diesel engines through the use of fuel additives. Advanced materials and composite materials with lightweight construction will greatly enhance the efficiency and environmental sustainability of surface, water and air transport. New polymer materials can increase the efficiency of existing methods for energy source production, e.g. adding polymer materials to oil wells to block water or to improve oil production.

New insulation materials in the household already allow the construction of three-litre houses, i.e. houses that consume less than three litres of fossil fuel per square metre per year (30 kWh/m$^2$). The aim is to develop this further to create the plus energy house, i.e. a house that produces more energy than it consumes. Here important products and technologies such as solar cells and active phase-changing materials (useful for controlling the climate within the house) play a vital role in saving energy. New nanoporous insulating materials can provide enhanced insulation, with a higher degree of energy conservation. Efficient lighting in the form of light emitting diodes could replace the light bulbs based on tungsten wire and fluorescent tubes. Heat and light management can be further supported through smart functional window coatings or layers. Semi-conducting polymers could save the environment and economies from the burden of corrosion.

Thermoelectric devices are solid-state systems that can convert heat into electricity. In the process they provide cooling and precise temperature control. Tiny dots of thermoelectrical material could convert the waste heat produced by automobiles or microprocessor chips to produce electrical energy and as a result cool them.

To achieve these goals a number of technologies need to be either improved or developed. A couple of examples are illustrated in the roadmap, including:

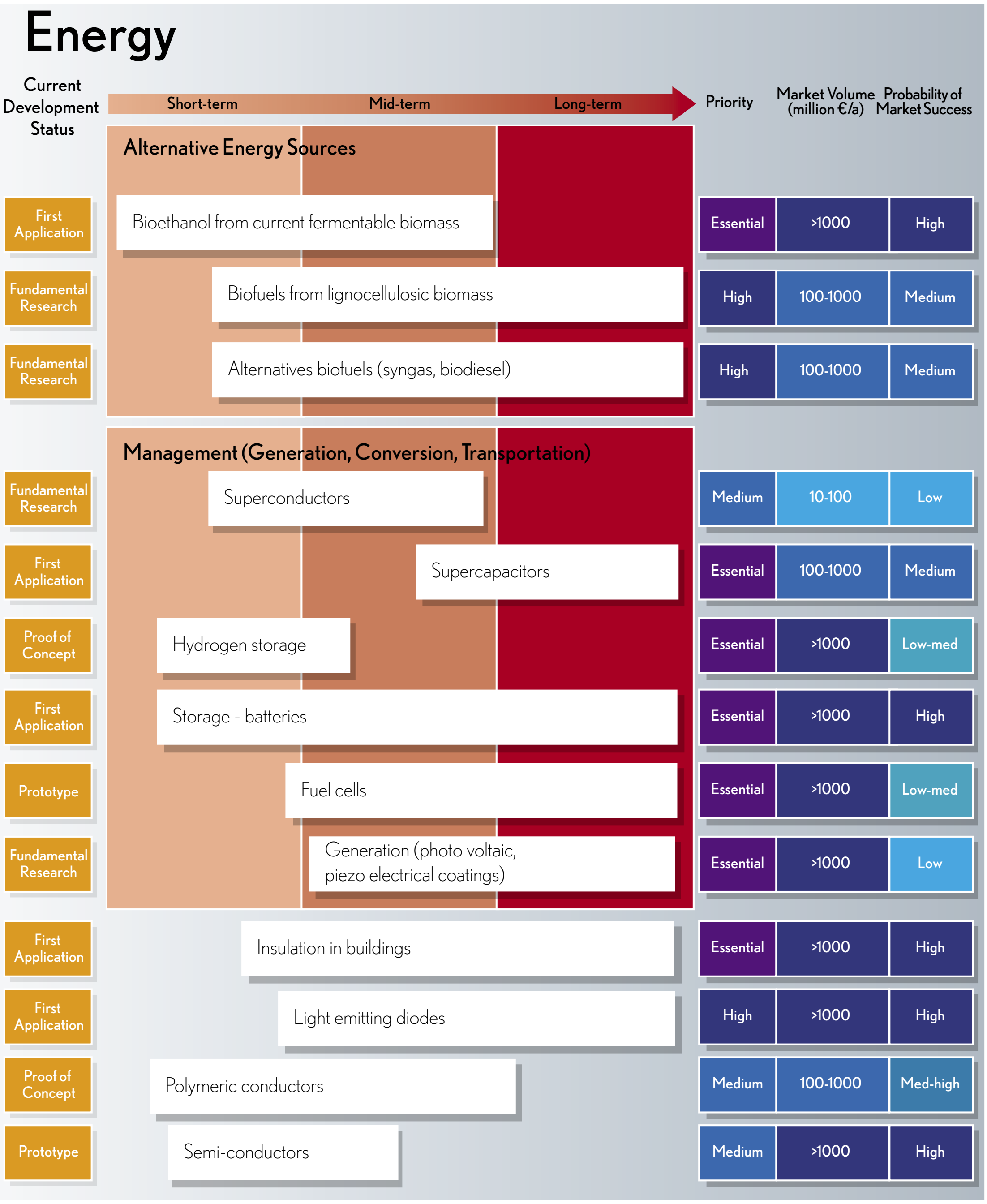
### Alternative sources

One of the most challenging tasks will be to adapt and transform the chemical industry's dependence on fossil fuels. There are three aspects that could be pursued. One is to reduce the dependence on oil as a raw material for chemicals by conversion to gas, coal or to biomass as a feedstock. This would require many technological adjustments to the production process, depending on the source being utilised. The second is related to this and is the utilisation of bioprocesses to generate biofuels from appropriate biomasses. The third set of technologies is that which enables the production of hydrogen in a clean form, including new catalysts.

### Management

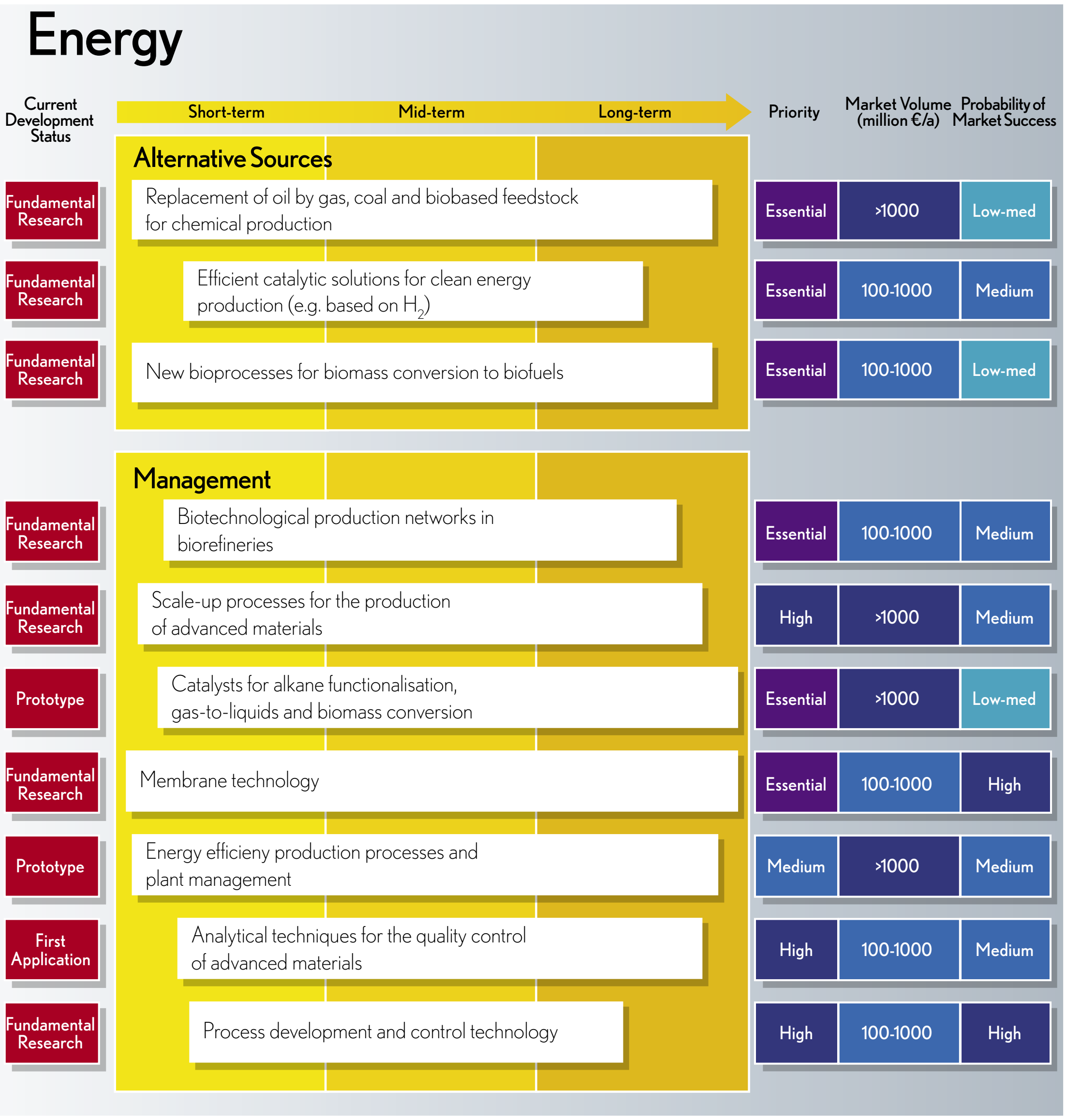
Various technologies could play a vital role in managing energy in the future, from making processes more efficient (catalysts, biomass conversion, plant management), to realising new developments (membranes for fuel cells, biorefineries). Associated with these is the appropriate development of scale-up production processes, control technologies and analytical techniques for the production of materials and for plant operation (control).

*Figure A.1: Products roadmap for energy*



| Current Development Status | Product | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| | **Alternative Energy Sources** | | | |
| First Application | Bioethanol from current fermentable biomass | Essential | >1000 | High |
| Fundamental Research | Biofuels from lignocellulosic biomass | High | 100-1000 | Medium |
| Fundamental Research | Alternatives biofuels (syngas, biodiesel) | High | 100-1000 | Medium |
| | **Management (Generation, Conversion, Transportation)** | | | |
| Fundamental Research | Superconductors | Medium | 10-100 | Low |
| First Application | Supercapacitors | Essential | 100-1000 | Medium |
| Proof of Concept | Hydrogen storage | Essential | >1000 | Low-med |
| First Application | Storage - batteries | Essential | >1000 | High |
| Prototype | Fuel cells | Essential | >1000 | Low-med |
| Fundamental Research | Generation (photo voltaic, piezo electrical coatings) | Essential | >1000 | Low |
| First Application | Insulation in buildings | Essential | >1000 | High |
| First Application | Light emitting diodes | High | >1000 | High |
| Proof of Concept | Polymeric conductors | Medium | 100-1000 | Med-high |
| Prototype | Semi-conductors | Medium | >1000 | High |

*Figure A.2: Technology development roadmap for energy*



# Energy

| Current Development Status | Short-term / Mid-term / Long-term | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| | **Alternative Sources** | | | |
| Fundamental Research | Replacement of oil by gas, coal and biobased feedstock for chemical production | Essential | >1000 | Low-med |
| Fundamental Research | Efficient catalytic solutions for clean energy production (e.g. based on $H_2$) | Essential | 100-1000 | Medium |
| Fundamental Research | New bioprocesses for biomass conversion to biofuels | Essential | 100-1000 | Low-med |
| | **Management** | | | |
| Fundamental Research | Biotechnological production networks in biorefineries | Essential | 100-1000 | Medium |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |
| Prototype | Catalysts for alkane functionalisation, gas-to-liquids and biomass conversion | Essential | >1000 | Low-med |
| Fundamental Research | Membrane technology | Essential | 100-1000 | High |
| Prototype | Energy efficieny production processes and plant management | Medium | >1000 | Medium |
| First Application | Analytical techniques for the quality control of advanced materials | High | 100-1000 | Medium |
| Fundamental Research | Process development and control technology | High | 100-1000 | High |

## 2

## Products and Technologies for the Electronics Industry - Communication, Information, Entertainment

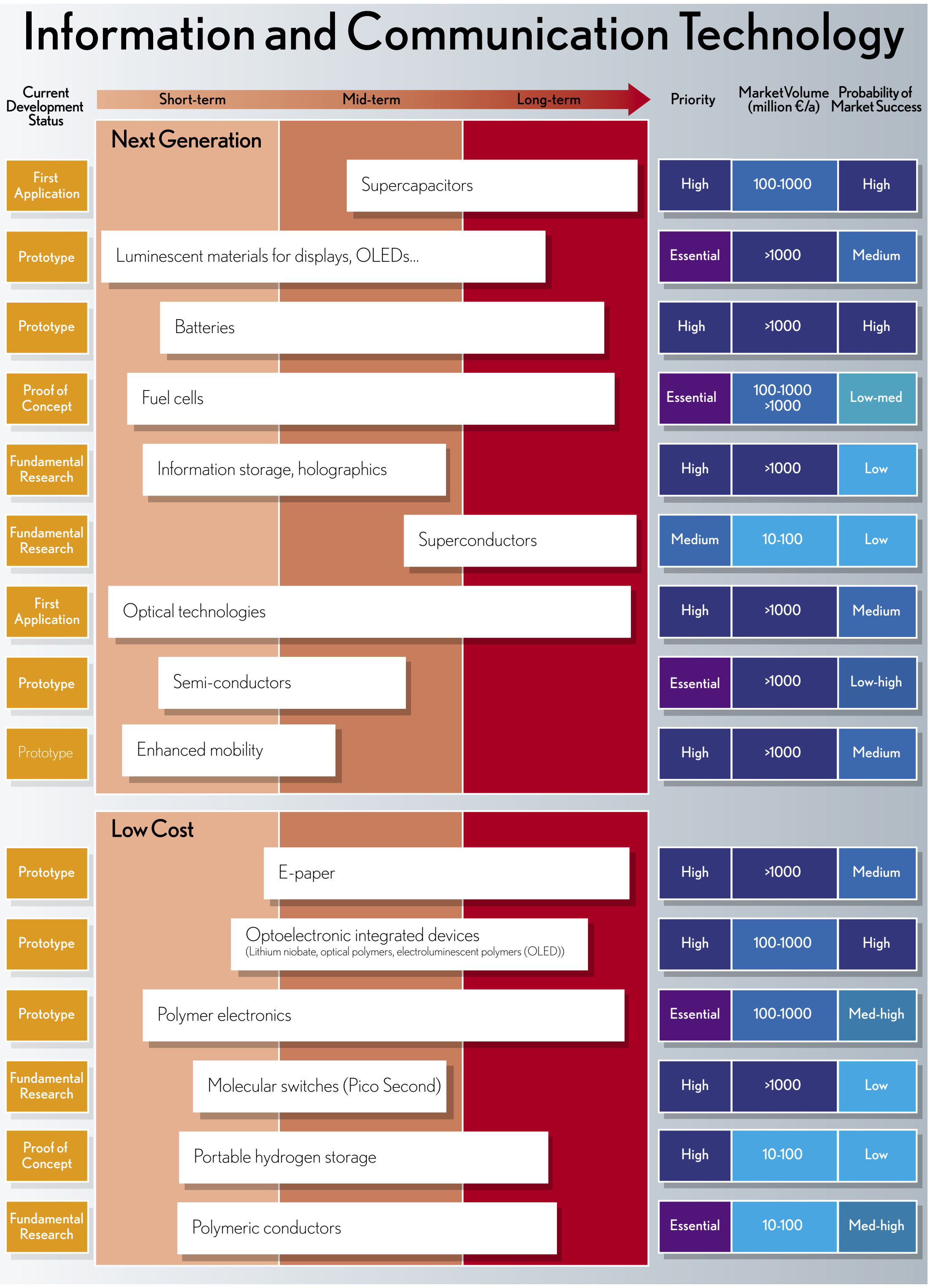
The electronics industry is one of the fastest changing and innovative industries in the world. A large portion of these changes can be attributed to the discovery and controlled manufacture of multi-functional materials, such as silicon-based semi-conductors, polycarbonates for optical-data storage and liquid crystals for displays. Therefore, further developments in the electronic industries will rely on research activities in material science to provide new products and technologies.

**The next generation and low cost**
New paradigms in the electronics industry will be the application of organic electronics, bulk-based 3D molecular electronics (for liquid crystalline displays), dye lasers, light-emitting diodes (for faster processors), plastic transistors and functional electronic devices that are able to use molecules as logic and memory elements, with switching times in the pico-second range. Supercapacitors and superconducting materials will boost the performance of high-end supercomputers.

An important factor that needs to be addressed is the cost of production and ultimately the cost for the end user. Here, advanced materials based on significantly cheaper raw materials, such as plastics or organic components, will play a significant role (OLEDs etc.). This could lead to new products such as e-paper, leading to new forms of newspapers, magazines and books. Production technologies need to be developed (illustrated below) that are more efficient and economic. The mobility and portability of new devices will be important; here, new forms of batteries and fuel cells will be a prerequisite. The storage of electronic information is a central theme, whether the medium is magnetic, holographic or optical; the storage capacities needed in the future will be enormous, due to the amounts of information being generated daily.

The emerging nanofabrication technologies, which lie beyond the optimisation of lithography techniques, require intensive research, in order to enable the production of new materials and products. Electron-beam nanolithography is a nanofabrication method, which has a higher resolution than current systems, enabling the production of structures down to 7 nm. Other currently emerging technologies are: the printing techniques (nanoimprint), where a stamp prepared using electron-beam nanolithography is applied to a polymer that is imprinting the desired nanopattern; and inking techniques, where the stamp is covered by an ink, that when deposited on a substrate creates the desired mask. Other emerging techniques are based on the bottom-up approach: where small structures are built up with atoms or molecules level by level. The first bottom-up method simply took advantage of the development of molecular electronic measurement tools, such as the Atomic Force Microscope and the Scanning Tunnel Microscope. New bottom-up nanofabrication techniques are based on the phenomena of self-assembly, where organic or inorganic molecules organise themselves under appropriate conditions into ordered structures, yielding a desired functionality.

*Figure A.3: Products roadmap for Information Communication Technology*

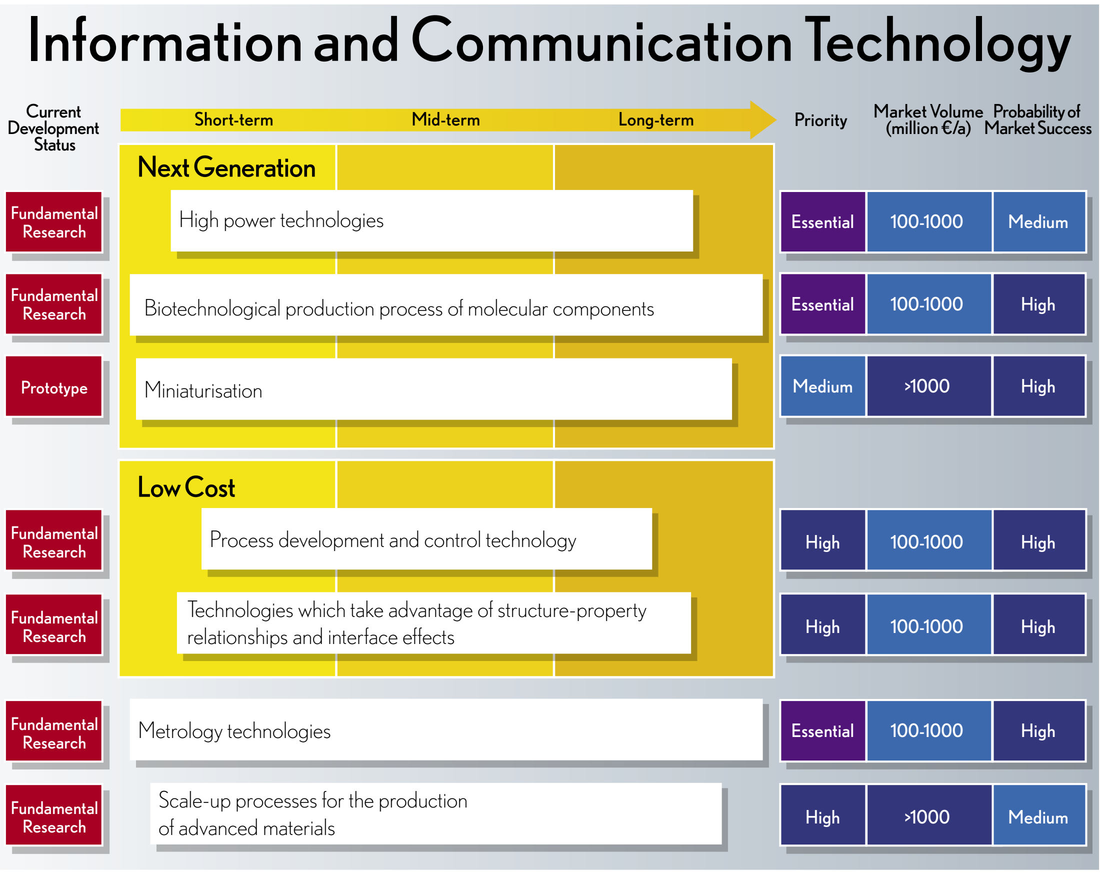


## Information and Communication Technology

| Current Development Status | Next Generation | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| First Application | Supercapacitors | High | 100-1000 | High |
| Prototype | Luminescent materials for displays, OLEDs... | Essential | >1000 | Medium |
| Prototype | Batteries | High | >1000 | High |
| Proof of Concept | Fuel cells | Essential | 100-1000<br>>1000 | Low-med |
| Fundamental Research | Information storage, holographics | High | >1000 | Low |
| Fundamental Research | Superconductors | Medium | 10-100 | Low |
| First Application | Optical technologies | High | >1000 | Medium |
| Prototype | Semi-conductors | Essential | >1000 | Low-high |
| Prototype | Enhanced mobility | High | >1000 | Medium |

| Current Development Status | Low Cost | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Prototype | E-paper | High | >1000 | Medium |
| Prototype | Optoelectronic integrated devices (Lithium niobate, optical polymers, electroluminescent polymers (OLED)) | High | 100-1000 | High |
| Prototype | Polymer electronics | Essential | 100-1000 | Med-high |
| Fundamental Research | Molecular switches (Pico Second) | High | >1000 | Low |
| Proof of Concept | Portable hydrogen storage | High | 10-100 | Low |
| Fundamental Research | Polymeric conductors | Essential | 10-100 | Med-high |

*Figure A.4: Technology development roadmap for Information Communication Technology*



**Information and Communication Technology**

| Current Development Status | | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| | **Next Generation** | | | |
| Fundamental Research | High power technologies | Essential | 100-1000 | Medium |
| Fundamental Research | Biotechnological production process of molecular components | Essential | 100-1000 | High |
| Prototype | Miniaturisation | Medium | >1000 | High |
| | **Low Cost** | | | |
| Fundamental Research | Process development and control technology | High | 100-1000 | High |
| Fundamental Research | Technologies which take advantage of structure-property relationships and interface effects | High | 100-1000 | High |
| Fundamental Research | Metrology technologies | Essential | 100-1000 | High |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |

## 3 Products and Technologies for Healthcare

The health, nutrition and agriculture sectors will benefit greatly from new products and technologies provided by material science. In the health sector, the scope covers new treatments through to medical devices, while in the fast moving consumer goods (FMCG), and the food and beverage industry, the benefits will come from new additives and preservatives. In the agricultural sector, the impact will be in new delivery systems for pesticides, nutrients or supplements.

**Home hospital**

One future vision is the idea of a home hospital. For this to be realised, products need to be developed that allow for the remote observation and diagnosis of patients. One can envisage intelligent clothes, made from functional textiles, which observe and record parameters, such as blood pressure, pulse, temperature, etc., and report these to a doctor. Developments such as lab on a chip for instant diagnosis, coupled with smart delivery systems, would enable treatment of diseases and illnesses at a very early stage. These could all be combined together into an implemented health system, where the doctor can remotely supervise his/her patients.

The challenges for the next century in healthcare are: an ever-increasing number of patients with allergic, inheritable or contagious diseases, cancers, the demographic trend to an older society and the exploding costs of healthcare. Nanotechnology could provide a means to cope with these challenges. Nanotechnology has the potential to revolutionise medical technologies and therapies to such an extent that its contribution will be crucial for future human health.

Nanoparticulate formulations will be one of the most important technological and scientific challenges in the fields of advanced food, drug and agricultural technologies. Exploitation of these nanoscale functionalities for new applications promises to have an immense impact in improved healthcare and quality of life, not only for the European Community, but also the rest of the world, in particularly the third world. This will be achieved through improved sustainability and protection of crops, effective drug applications, faster and non-invasive medical diagnostics and treatments, and through a well-balanced nutritional diet adjusted to the needs of modern societies. Irrespective of the broad nature of these applications, the technologies needed here encompass similar and complementary generic knowledge and expertise.

The fundamental understanding of the interactions of artificial materials with biological interfaces should result in a revolution, leading to novel delivery methods, biocompatible materials for bone reconstruction, tissue engineering and increased bioavailability of nutrients (vitamins, minerals, essential amino acids etc.).

The increasing percentage of elderly people in both the western and eastern world will require improved and innovative novel drug treatments with respect to efficacy and drug safety. Nanoscience-based materials are considered as one of the keys in improving drug substance properties. As drugs will in most cases not be administered per se, but will need special formulations for optimised applications and treatments, novel excipients and particle size engineering efforts, based on new nanotechnologies, resulting in very fine particles with specific surfaces or cavities, will impact pharmaceutical research and drug development. Improved bioavailability after administration by mouth or lungs will result in lower drug substance demands, and therefore a lower demand for starting materials for drug production, and consequently lower energy consumption.

Formulation properties with increased bioavailability and intelligent release profiles could lead to drug release along circadian rhythms. It is envisaged that drugs might circulate inside nanotubes for days within the body, releasing the active ingredients perhaps due to the action of a biological species over an extended time. Nanotubes or special surfaces as carriers for drug molecules will potentially improve the distribution in the body, increasing drug stability, influencing drug absorption in the gut and from the lung, and thereby protecting drugs from rapid enzymatic biotransformation or from being affected by other clearance mechanisms. As the potency of drug molecules continuously increases and the doses a patient requires decreases into the mg and µg range, improved bioavailability along with improved potency, and novel nanostructure-based formulations could lead to the development of µg and sub µg doses for very efficient treatments. The improvement of conventionally fabricated tablets by new surface coatings and coating techniques achieved through optimised formulation research, could result in new avenues towards improved and efficacious drug treatments.

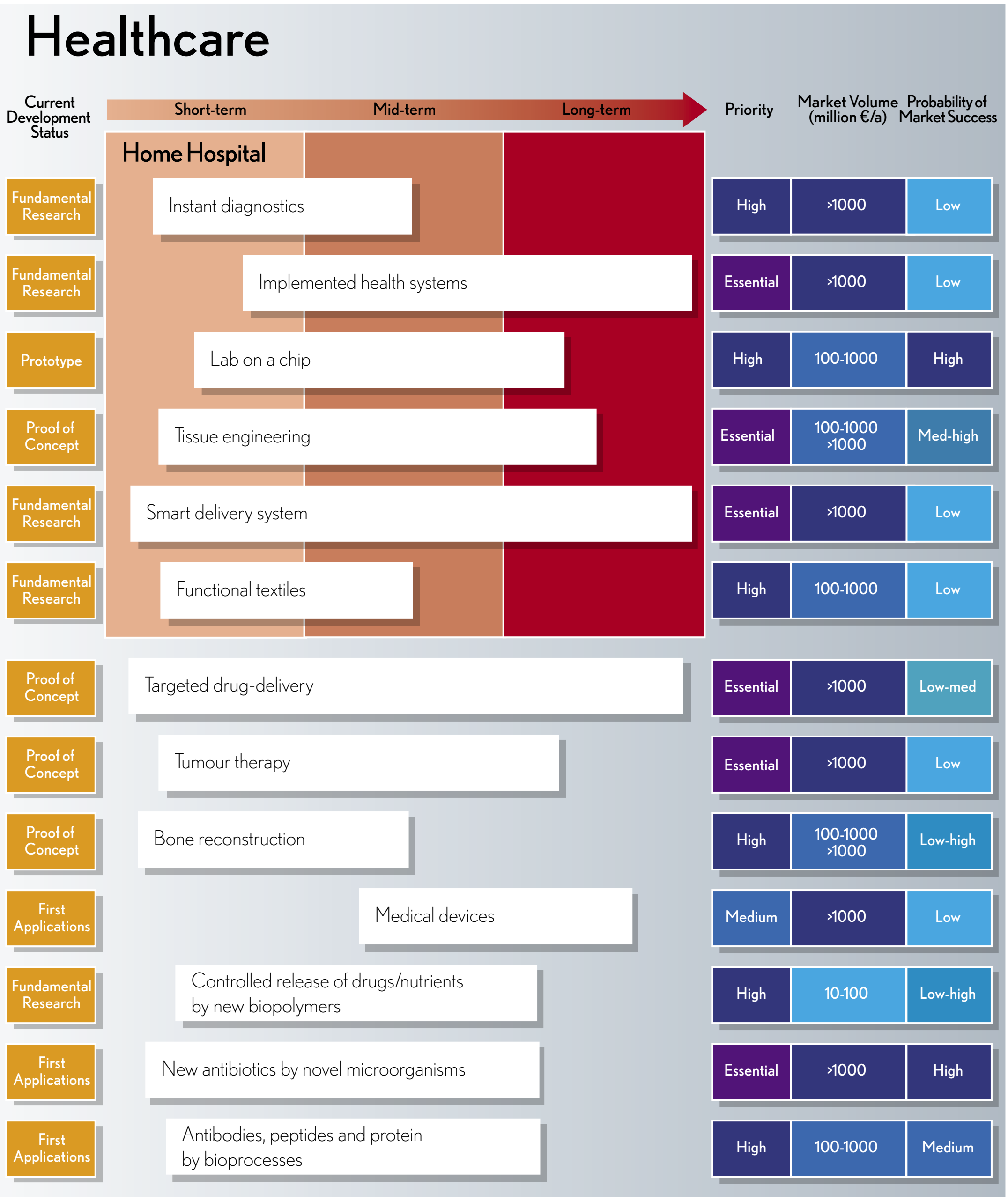
Faster and more reliable diagnostics can be developed using new types of biosensors and biochips for fast vectorial testing of biological substances. New contrast imaging agents for imaging technologies like Magnetic Resonance Imaging (MRI) and Computer Tomography (CT), which are patient-friendly and provide better resolution leading to earlier identification of diseases, are important. To be able to grow tissue for transplantation (tissue engineering) is another vital healthcare product which needs to be pursued.

The production of new antibiotics and antibodies through fermentation, or through other as yet undiscovered biotechnological processes, will lead to a new age in the treatment of diseases. The further development of novel fermentation processes and biocatalytic transformations in particular is of great importance.

To summarise, the following healthcare and medicine topics for the 21st century will be impacted by nanotechnology:

- Early cancer diagnostic.
- Improved imaging techniques, e.g. nanoparticles as reporter platforms and contrast-enhancing agents.
- Intra-cellular drug and gene delivery.
- Self-assembling nanosystems.
- Nanoparticles for delivery of electromagnetic energy for hyperthermia and thermal ablation of tumours.
- Functionalisation and preparation of nanoparticles like polymer particles, lipid nanoparticles, metal nanoparticles or magnetic nanoparticles.
- Nanotechnology for detection of biomarkers.
- Design and synthesis of functional cosmetics, e.g. sun protection.
- Modelling and simulation of reactions, transportation and processes of nanoparticles *in-vitro* environment.

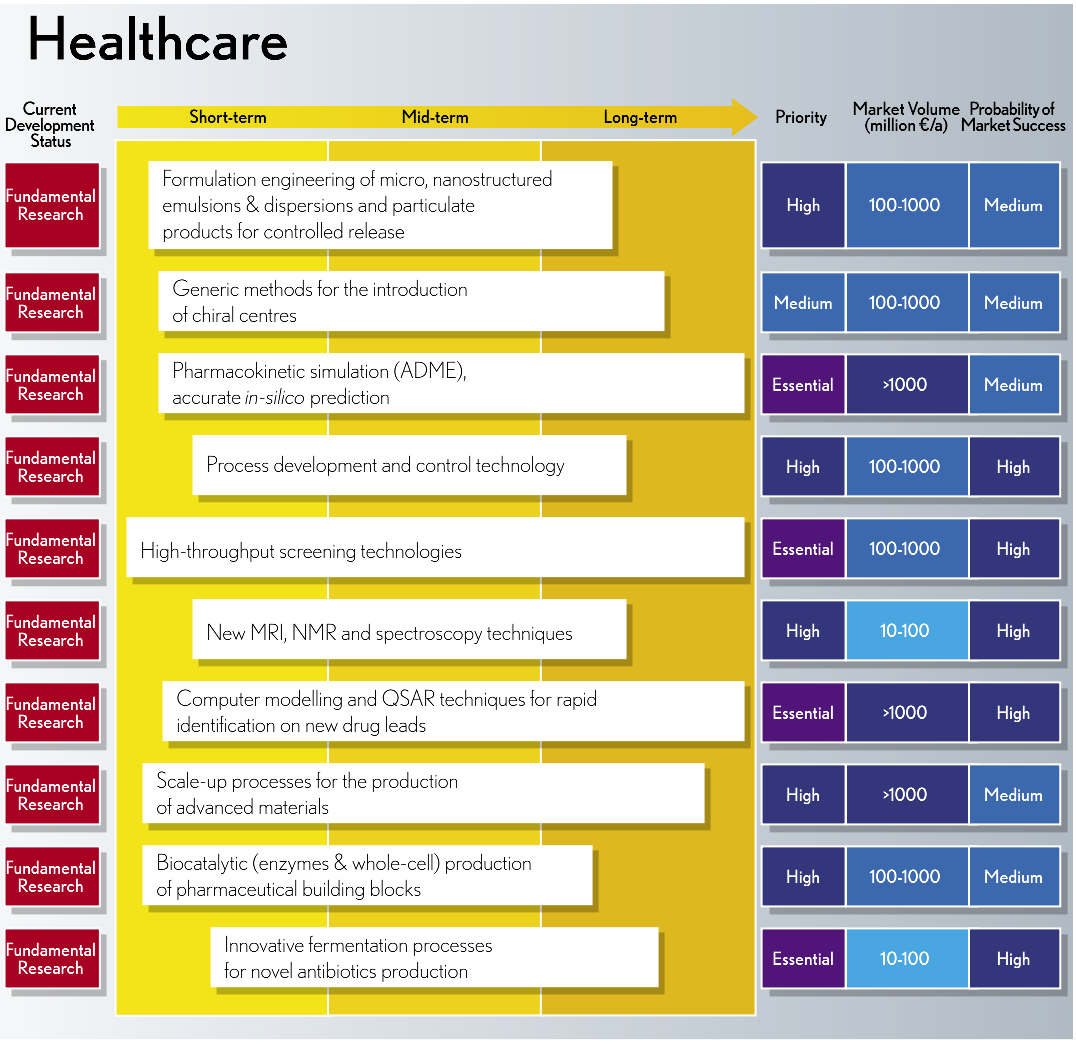
*Figure A.5: Products roadmap for healthcare*



## Healthcare

| Current Development Status | Product | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| | **Home Hospital** | | | |
| Fundamental Research | Instant diagnostics | High | >1000 | Low |
| Fundamental Research | Implemented health systems | Essential | >1000 | Low |
| Prototype | Lab on a chip | High | 100-1000 | High |
| Proof of Concept | Tissue engineering | Essential | 100-1000<br>>1000 | Med-high |
| Fundamental Research | Smart delivery system | Essential | >1000 | Low |
| Fundamental Research | Functional textiles | High | 100-1000 | Low |
| Proof of Concept | Targeted drug-delivery | Essential | >1000 | Low-med |
| Proof of Concept | Tumour therapy | Essential | >1000 | Low |
| Proof of Concept | Bone reconstruction | High | 100-1000<br>>1000 | Low-high |
| First Applications | Medical devices | Medium | >1000 | Low |
| Fundamental Research | Controlled release of drugs/nutrients by new biopolymers | High | 10-100 | Low-high |
| First Applications | New antibiotics by novel microorganisms | Essential | >1000 | High |
| First Applications | Antibodies, peptides and protein by bioprocesses | High | 100-1000 | Medium |

*Figure A.6: Technology development roadmap for healthcare*



Healthcare

| Current Development Status | Short-term Mid-term Long-term | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Fundamental Research | Formulation engineering of micro, nanostructured emulsions & dispersions and particulate products for controlled release | High | 100-1000 | Medium |
| Fundamental Research | Generic methods for the introduction of chiral centres | Medium | 100-1000 | Medium |
| Fundamental Research | Pharmacokinetic simulation (ADME), accurate *in-silico* prediction | Essential | >1000 | Medium |
| Fundamental Research | Process development and control technology | High | 100-1000 | High |
| Fundamental Research | High-throughput screening technologies | Essential | 100-1000 | High |
| Fundamental Research | New MRI, NMR and spectroscopy techniques | High | 10-100 | High |
| Fundamental Research | Computer modelling and QSAR techniques for rapid identification on new drug leads | Essential | >1000 | High |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |
| Fundamental Research | Biocatalytic (enzymes & whole-cell) production of pharmaceutical building blocks | High | 100-1000 | Medium |
| Fundamental Research | Innovative fermentation processes for novel antibiotics production | Essential | 10-100 | High |

## 4 Products and Technologies for the Enhancement of the Quality of Life

Some of the products and technologies mentioned in the previous section also have an application in improving Quality of Life (QoL). Healthcare examples include the stable formulation of vitamins or other nutrients with increased bioavailability, and new cosmetic and personal care systems with enhanced activity. In the sphere of Information CommunicationTechnology, new systems to enhance mobility, i.e. smaller and longer-lasting batteries for cellular phones and laptops, new low-energy display components where the quality of the image does not depend on the viewing angle, and electronic paper as an alternative to books, newspapers and magazines, could enhance the quality of life of European citizens.

### Eco-efficiency

A very important area is the development of functional and interactive textiles that are self-cleaning, adaptive to the external environment (e.g. change colour, regulate ambient temperature, incident light, etc.) and provide protection against weather or other extreme conditions. Related to this is the development of efficient and environmentally-friendly domestic laundry processes to clean modern textiles. The development of biofibres and the incorporation of enzymes into detergents is one possible solution.

An area that promises the largest impact on the QoL is the construction and building sector. For example, the plus energy house, which, through the use of intelligent materials and technologies, consumes less energy than it produces, allowing the excess to be transferred back into the power grids. Other aspects are the development of new building materials based on nanotechnologies (nanostructured materials such as insulators, etc.), materials from renewable sources (polymers) and efficient lighting (through the use of organic and inorganic LEDs).

Another area is the development of smart surfaces that can respond to various external stimuli to detect toxic chemicals or bacteria and bind and destroy them, or have anti-fouling and anti-corrosion activities, etc.

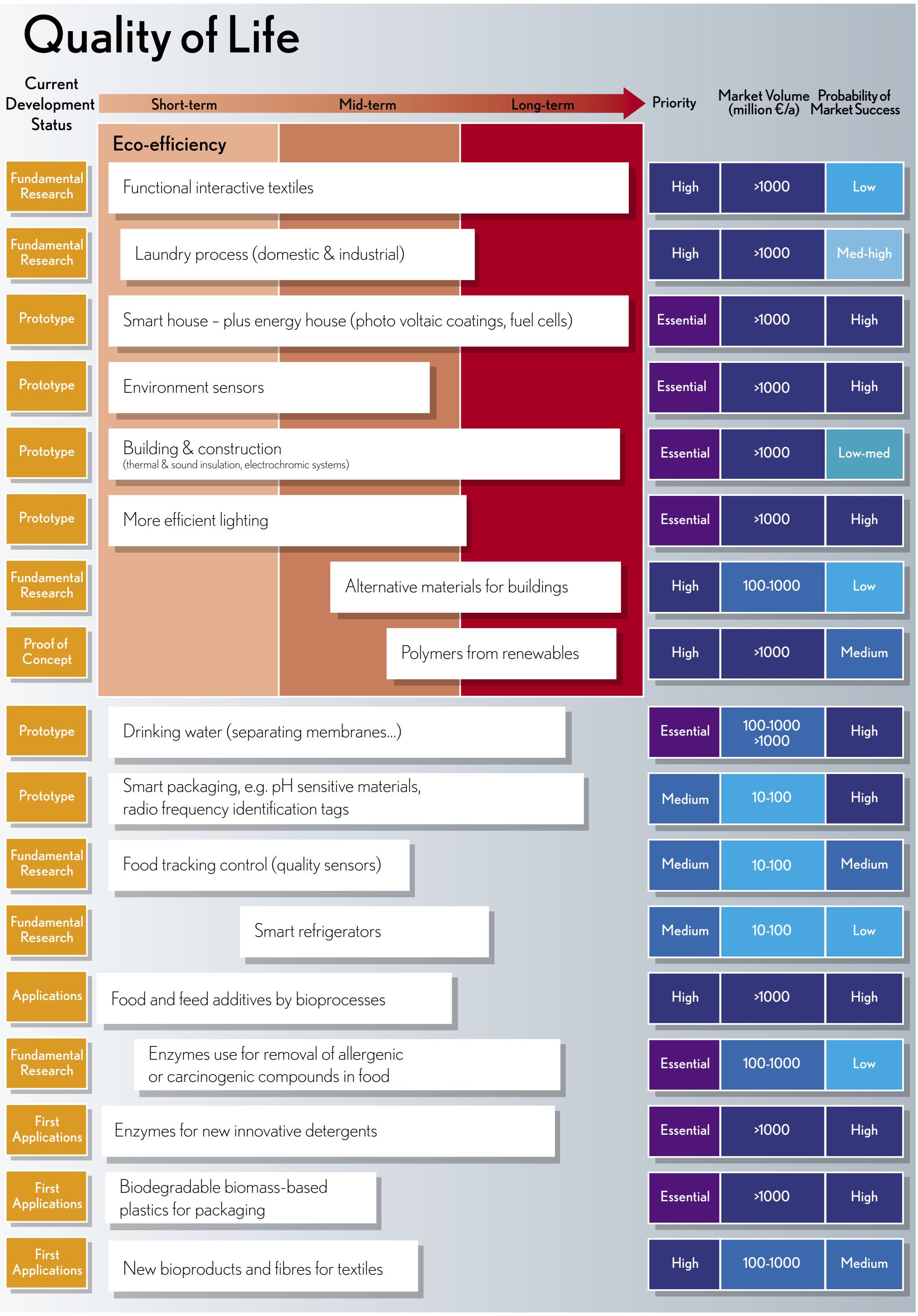
### Other priorities

One of the most pressing issues facing the world is the sustainable supply of fresh drinking water. Through the development of new types of filtering processes and membrane technologies, the efficient and cost-effective transformation of seawater into potable water could be realised.

The implementation of food tracking controls and smart packaging materials will allow better management of food stocks in stores, and allow the customer to determine the quality of the product at a glance. The development of smart refrigerators, which are energy-efficient, able to monitor the quality of food kept within them, and to issue a warning when the food begins to spoil, would be advantageous. An extra feature would be for the fridge to monitor the presence of a standard set of food items, and to order any of these when they run out.

A market sector of huge importance is that of the food and feed sector. Here, advances in the nature and types of additives will pose a significant advantage to mankind.

*Figure A.7: Products roadmap for enhancement of the quality of life*

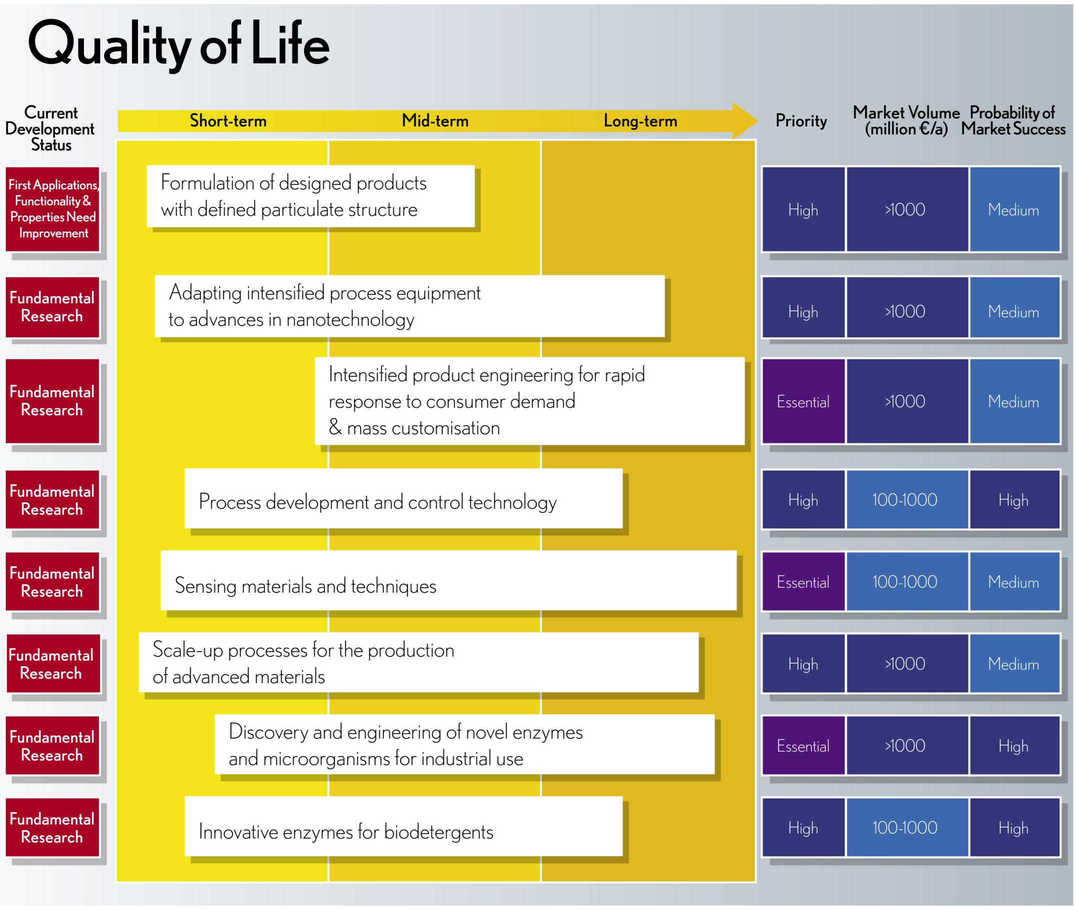


## Quality of Life

Short-term Mid-term Long-term

| Current Development Status | | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| | **Eco-efficiency** | | | |
| Fundamental Research | Functional interactive textiles | High | >1000 | Low |
| Fundamental Research | Laundry process (domestic & industrial) | High | >1000 | Med-high |
| Prototype | Smart house – plus energy house (photo voltaic coatings, fuel cells) | Essential | >1000 | High |
| Prototype | Environment sensors | Essential | >1000 | High |
| Prototype | Building & construction (thermal & sound insulation, electrochromic systems) | Essential | >1000 | Low-med |
| Prototype | More efficient lighting | Essential | >1000 | High |
| Fundamental Research | Alternative materials for buildings | High | 100-1000 | Low |
| Proof of Concept | Polymers from renewables | High | >1000 | Medium |
| Prototype | Drinking water (separating membranes...) | Essential | 100-1000<br>>1000 | High |
| Prototype | Smart packaging, e.g. pH sensitive materials, radio frequency identification tags | Medium | 10-100 | High |
| Fundamental Research | Food tracking control (quality sensors) | Medium | 10-100 | Medium |
| Fundamental Research | Smart refrigerators | Medium | 10-100 | Low |
| Applications | Food and feed additives by bioprocesses | High | >1000 | High |
| Fundamental Research | Enzymes use for removal of allergenic or carcinogenic compounds in food | Essential | 100-1000 | Low |
| First Applications | Enzymes for new innovative detergents | Essential | >1000 | High |
| First Applications | Biodegradable biomass-based plastics for packaging | Essential | >1000 | High |
| First Applications | New bioproducts and fibres for textiles | High | 100-1000 | Medium |

*Figure A.8: Technology development roadmap for the quality of life*



## Quality of Life

Short-term Mid-term Long-term

| Current Development Status | | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| First Applications, Functionality & Properties Need Improvement | Formulation of designed products with defined particulate structure | High | >1000 | Medium |
| Fundamental Research | Adapting intensified process equipment to advances in nanotechnology | High | >1000 | Medium |
| Fundamental Research | Intensified product engineering for rapid response to consumer demand & mass customisation | Essential | >1000 | Medium |
| Fundamental Research | Process development and control technology | High | 100-1000 | High |
| Fundamental Research | Sensing materials and techniques | Essential | 100-1000 | Medium |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |
| Fundamental Research | Discovery and engineering of novel enzymes and microorganisms for industrial use | Essential | >1000 | High |
| Fundamental Research | Innovative enzymes for biodetergents | High | 100-1000 | High |

# 5 Products and Technologies for Citizen Protection

The US government awarded more than $28 billion to state and local governments to protect the US (The Department of Homeland Security (DHS) Appropriations Act) in 2005. This enormous amount of funding for security-related topics underpins the interest and the particular importance of citizen protection in the USA. Citizen protection is also a relevant topic in Europe.

### Alarm systems

Smart surfaces (functionalised polymers) that can respond to various external stimuli can be adapted to be part of an early warning system which detects toxic chemicals, binds and destroys them. They can also be used as pressure sensors in glass windows or in carpets to detect intruders. Additional sensor developments for the fast, cheap and accurate testing for explosives, radiation sources, weapons of mass destruction, and food/water contamination are needed. Windows, which can change their opacity at the touch of a button, or in response to a sensor or an alarm, are desirable as a security feature.

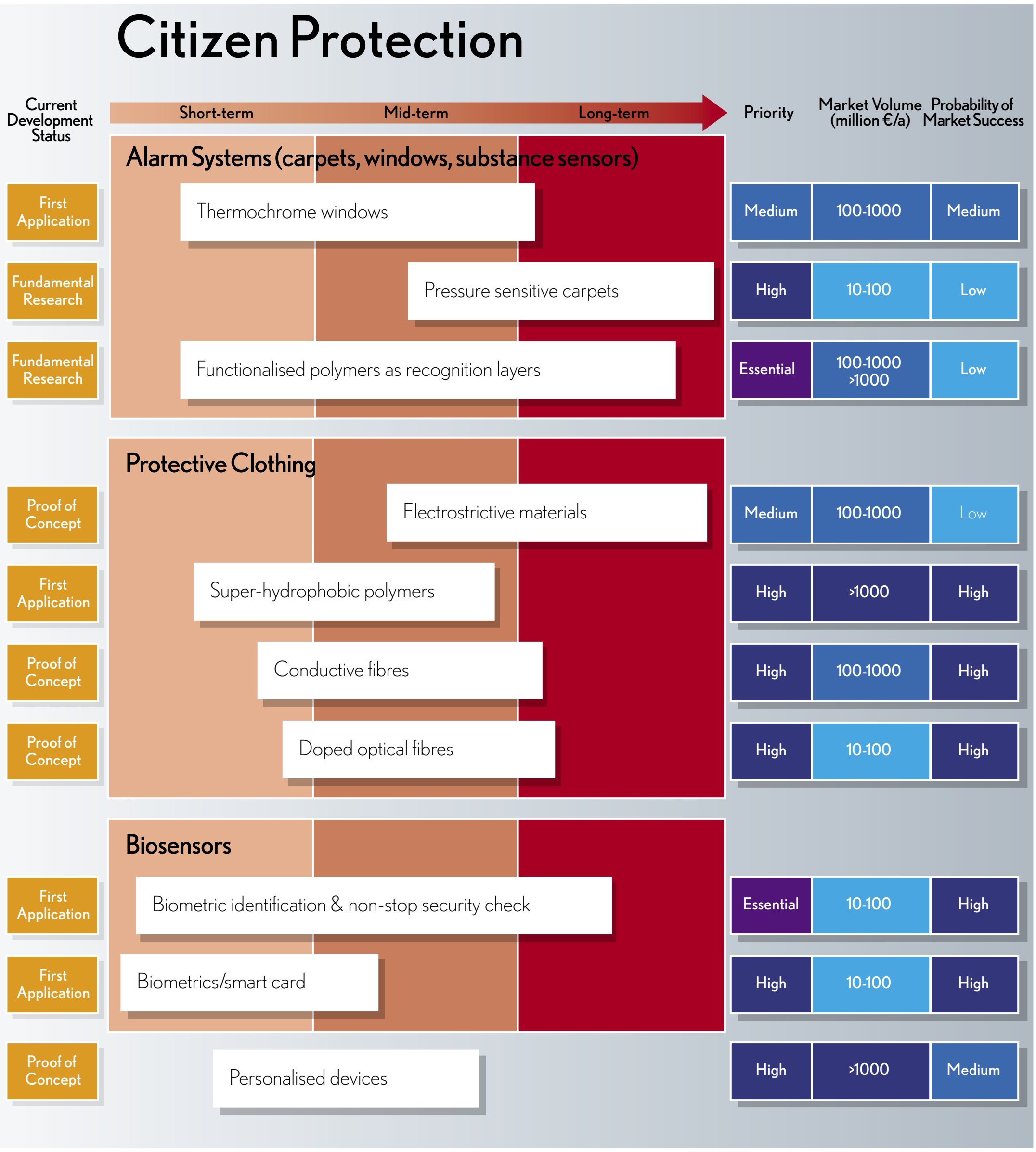
### Protective clothing

New textile materials than can protect persons and possessions exposed to extreme conditions, such as accidents or natural disasters, will become ever more important. Extreme climatic conditions have caused enormous personal and economic loss in Europe in the last few years. Examples include the flood catastrophe in Germany in 2001 and the fires that devastated regions in Spain, Portugal and Greece in 2003. The development of textiles made from nanomaterials, such as functional fibres (for the inclusion of devices), or from non-woven materials or nanotubes, are of high social interest.

### Biosensors

To enable quick and easy (non-stop) progression through airport security, the development of biometric identification technologies needs to be further pursued. These biometric data could also be stored on new forms of Smart Cards.

*Figure A.9: Products roadmap for citizen protection*



Citizen Protection

**Alarm Systems (carpets, windows, substance sensors)**

| Current Development Status | Product | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| First Application | Thermochrome windows | Medium | 100-1000 | Medium |
| Fundamental Research | Pressure sensitive carpets | High | 10-100 | Low |
| Fundamental Research | Functionalised polymers as recognition layers | Essential | 100-1000<br>>1000 | Low |

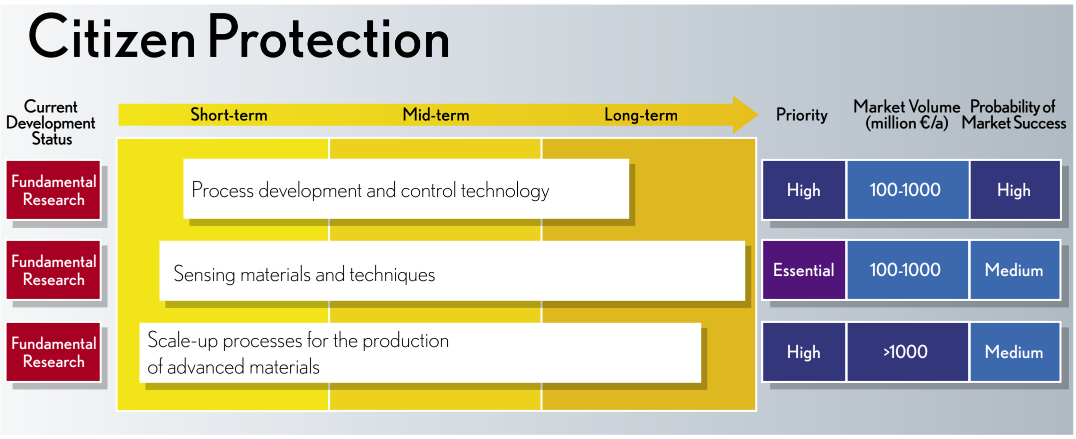
**Protective Clothing**

| Current Development Status | Product | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Proof of Concept | Electrostrictive materials | Medium | 100-1000 | Low |
| First Application | Super-hydrophobic polymers | High | >1000 | High |
| Proof of Concept | Conductive fibres | High | 100-1000 | High |
| Proof of Concept | Doped optical fibres | High | 10-100 | High |

**Biosensors**

| Current Development Status | Product | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| First Application | Biometric identification & non-stop security check | Essential | 10-100 | High |
| First Application | Biometrics/smart card | High | 10-100 | High |
| Proof of Concept | Personalised devices | High | >1000 | Medium |

*Figure A.10: Technology development roadmap for citizen protection*



## Citizen Protection

| Current Development Status | Short-term | Mid-term | Long-term | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|---|---|
| Fundamental Research | Process development and control technology | | | High | 100-1000 | High |
| Fundamental Research | Sensing materials and techniques | | | Essential | 100-1000 | Medium |
| Fundamental Research | Scale-up processes for the production of advanced materials | | | High | >1000 | Medium |

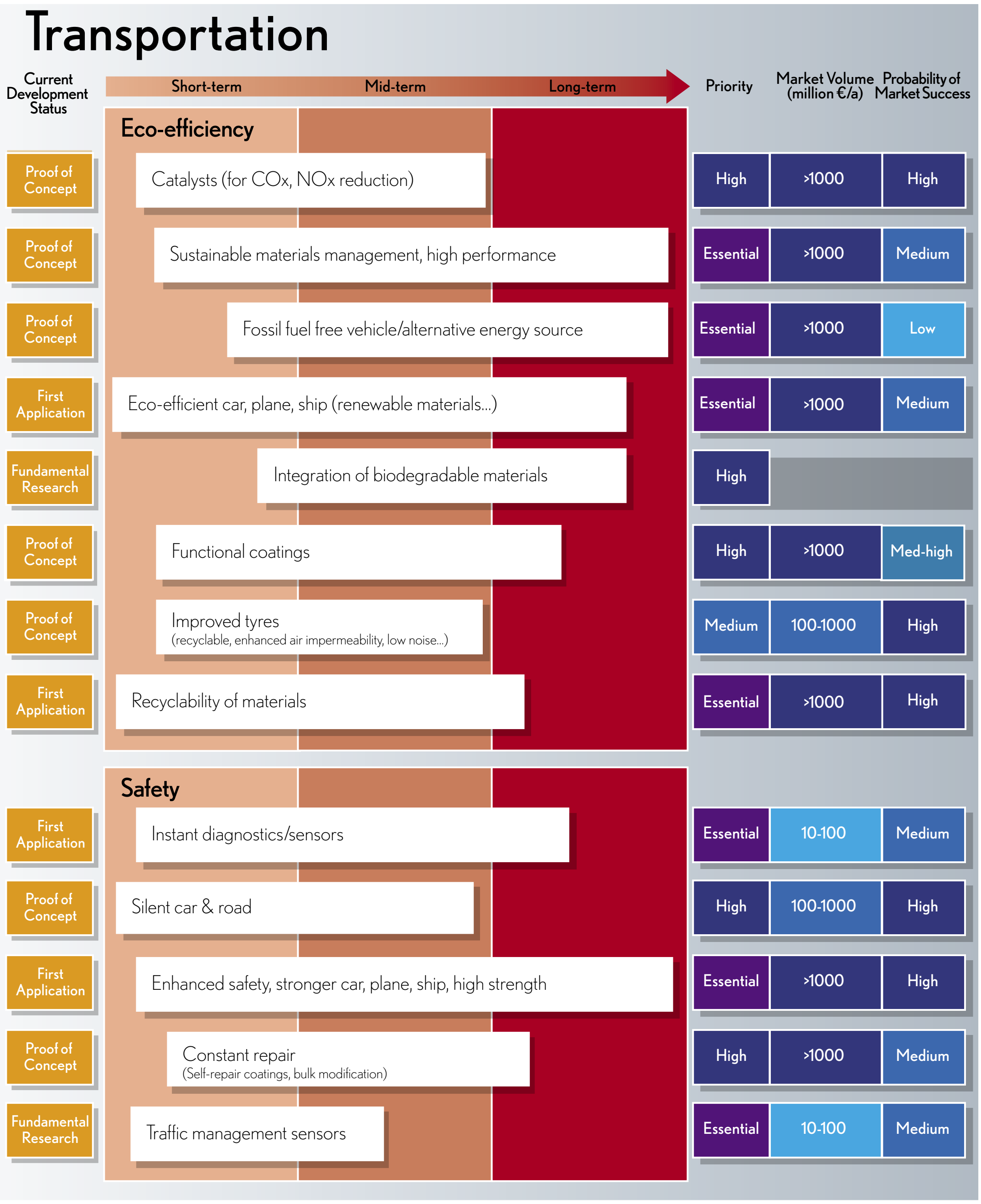
## 6 Products and Technologies for Transportation and Mobility

With the ever-increasing demands for personal mobility and a world shortage of fossil fuels, there is a great need to develop fossil fuel-free vehicles, eco-friendly alternative transport methods and new energy sources. The projected numbers of privately owned vehicles are set to continue to increase and therefore systems for effective traffic management are necessary. There is also the concurrent need to develop new catalytic converters for the greenhouse gases produced by vehicles. To enhance the security of road users, new driver aids need to be developed, including instant diagnostic systems. Vehicles composed of new materials with improved recyclability and biodegradability will benefit the environment, as will the ability to renew used parts and incorporate them into new vehicles. Such technologies will lead to eco-efficient cars, planes and ships.

To lessen the burden on the environment in the short- to medium-term, efforts should be concentrated on developing:

- Fuels from renewable sources, such as bioethanol and biodiesel.
- Recyclable and energy-efficient tyres have low friction but high grip, and reduce noise pollution.
- New functional coatings for vehicles that reduce air resistance (or water resistance) and therefore lead to lower fuel usage and thereby reduce the pollution of the environment.
- Self-cleaning long-lasting coatings with high scratch resistance and weatherability which could moderate against the need for paints currently used, for example, to prevent corrosion and water damage to ships that have to be renewed on a regular basis.

*Figure A.11: Products roadmap for transportation*



## Transportation

Short-term → Mid-term → Long-term

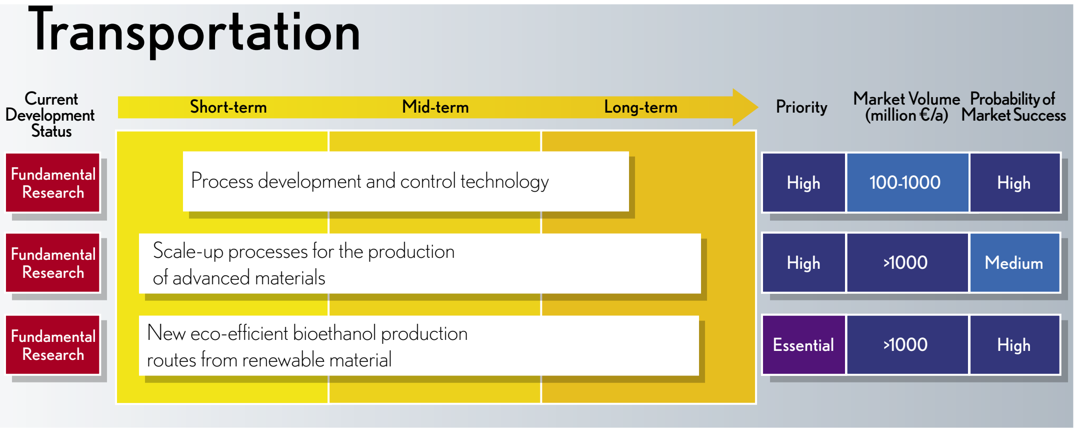
### Eco-efficiency

| Current Development Status | | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Proof of Concept | Catalysts (for COx, NOx reduction) | High | >1000 | High |
| Proof of Concept | Sustainable materials management, high performance | Essential | >1000 | Medium |
| Proof of Concept | Fossil fuel free vehicle/alternative energy source | Essential | >1000 | Low |
| First Application | Eco-efficient car, plane, ship (renewable materials...) | Essential | >1000 | Medium |
| Fundamental Research | Integration of biodegradable materials | High | | |
| Proof of Concept | Functional coatings | High | >1000 | Med-high |
| Proof of Concept | Improved tyres (recyclable, enhanced air impermeability, low noise...) | Medium | 100-1000 | High |
| First Application | Recyclability of materials | Essential | >1000 | High |

### Safety

| Current Development Status | | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| First Application | Instant diagnostics/sensors | Essential | 10-100 | Medium |
| Proof of Concept | Silent car & road | High | 100-1000 | High |
| First Application | Enhanced safety, stronger car, plane, ship, high strength | Essential | >1000 | High |
| Proof of Concept | Constant repair (Self-repair coatings, bulk modification) | High | >1000 | Medium |
| Fundamental Research | Traffic management sensors | Essential | 10-100 | Medium |

*Figure A.12: Technology development roadmap for transportation*



## Transportation

| Current Development Status | Short-term – Mid-term – Long-term | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Fundamental Research | Process development and control technology | High | 100-1000 | High |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |
| Fundamental Research | New eco-efficient bioethanol production routes from renewable material | Essential | >1000 | High |

# 7 Technologies for Eco-efficiency and the Environment

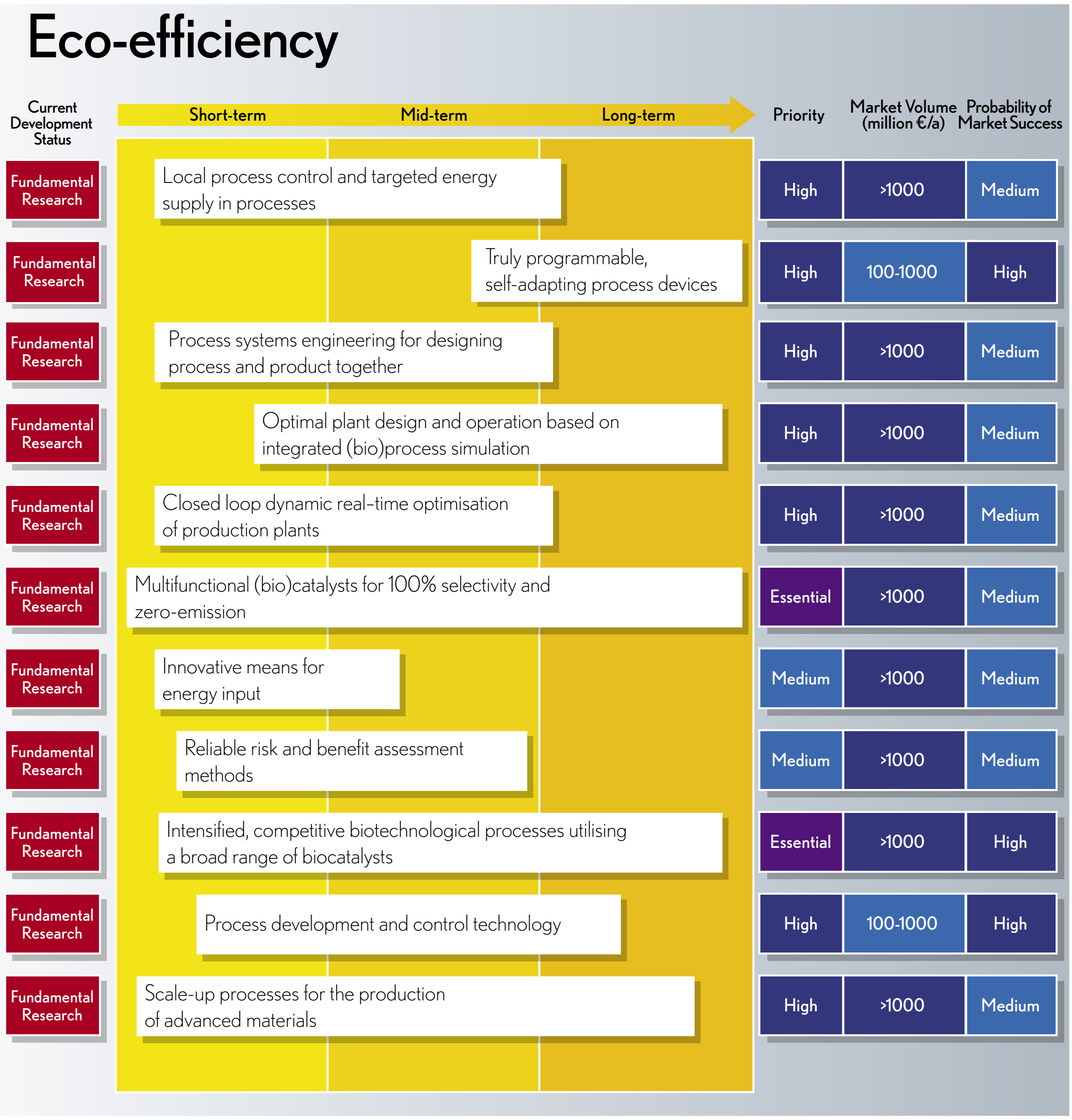
Concerns about the increasing environmental impact of human culture on the world environment have made the issues of eco-efficiency and environmental sustainability important political topics. To illustrate how SusChem and its stakeholders are addressing these concerns, the following technologies, some of which have already been mentioned in the previous sections, are highlighted below.

An important step to be undertaken is to achieve complete biodegradability of all new products, or at least to build in properties that prevent serious environmental impact. For production processes, low environmental impact could be achieved through the development of biosolvents and closed loop biorefineries that produce no waste. Very efficient biocatalysts are needed to make these processes very selective and at the same time economically competitive.

The energy needed for industrial processes represents a significant part of the overall energy requirement in Europe. Better process control and closed energy loops in processes, a locally targeted energy supply, as well as innovative forms of energy supply will increase the eco-efficiency of current production processes.

Chemistry is essential in a wide variety of environmental technologies. Water and soil treatment is only one point where, for example, catalysis can greatly enhance the remediation of contaminated water or soil. Also, methods to capture and separate $CO_2$ from exhaust gases from process and power plants are needed and can be achieved through new technology developments.

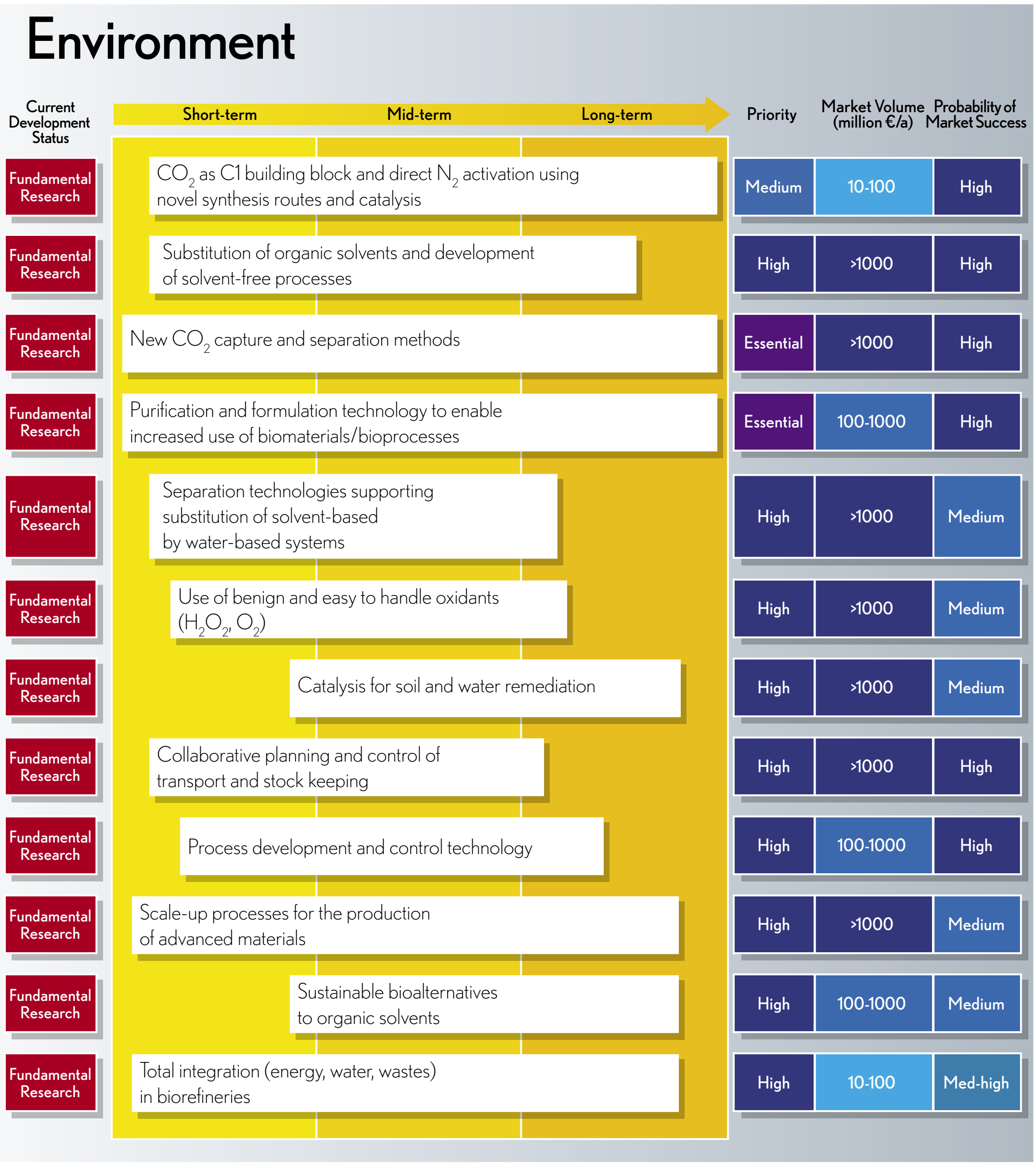
Figure A.13: Technology development roadmap for eco-efficiency



## Eco-efficiency

| Current Development Status | Short-term Mid-term Long-term | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Fundamental Research | Local process control and targeted energy supply in processes | High | >1000 | Medium |
| Fundamental Research | Truly programmable, self-adapting process devices | High | 100-1000 | High |
| Fundamental Research | Process systems engineering for designing process and product together | High | >1000 | Medium |
| Fundamental Research | Optimal plant design and operation based on integrated (bio)process simulation | High | >1000 | Medium |
| Fundamental Research | Closed loop dynamic real-time optimisation of production plants | High | >1000 | Medium |
| Fundamental Research | Multifunctional (bio)catalysts for 100% selectivity and zero-emission | Essential | >1000 | Medium |
| Fundamental Research | Innovative means for energy input | Medium | >1000 | Medium |
| Fundamental Research | Reliable risk and benefit assessment methods | Medium | >1000 | Medium |
| Fundamental Research | Intensified, competitive biotechnological processes utilising a broad range of biocatalysts | Essential | >1000 | High |
| Fundamental Research | Process development and control technology | High | 100-1000 | High |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |

Figure A.14: Technology development roadmap for environment



# Environment

| Current Development Status | Short-term Mid-term Long-term | Priority | Market Volume (million €/a) | Probability of Market Success |
|---|---|---|---|---|
| Fundamental Research | $CO_2$ as C1 building block and direct $N_2$ activation using novel synthesis routes and catalysis | Medium | 10-100 | High |
| Fundamental Research | Substitution of organic solvents and development of solvent-free processes | High | >1000 | High |
| Fundamental Research | New $CO_2$ capture and separation methods | Essential | >1000 | High |
| Fundamental Research | Purification and formulation technology to enable increased use of biomaterials/bioprocesses | Essential | 100-1000 | High |
| Fundamental Research | Separation technologies supporting substitution of solvent-based by water-based systems | High | >1000 | Medium |
| Fundamental Research | Use of benign and easy to handle oxidants ($H_2O_2$, $O_2$) | High | >1000 | Medium |
| Fundamental Research | Catalysis for soil and water remediation | High | >1000 | Medium |
| Fundamental Research | Collaborative planning and control of transport and stock keeping | High | >1000 | High |
| Fundamental Research | Process development and control technology | High | 100-1000 | High |
| Fundamental Research | Scale-up processes for the production of advanced materials | High | >1000 | Medium |
| Fundamental Research | Sustainable bioalternatives to organic solvents | High | 100-1000 | Medium |
| Fundamental Research | Total integration (energy, water, wastes) in biorefineries | High | 10-100 | Med-high |

# Industrial Biotechnology

## 1 Products of Industrial Biotechnology

The potential of Industrial Biotechnology (IB) lies in the ability to replace classical chemical production processes and to facilitate the production of new products. It is undisputed that, particularly in the area of bulk and fine chemicals production, the use of biotechnological processes is attractive since:

- Biotechnological processes are usually distinguished by their high specificity (relating to the conversion of substrates) and selectivity (relating to the product spectrum).
- Biotechnological processes often use renewable resources as raw materials, thus contributing to the much discussed sustainability of products and processes.
- Biotechnological processes can be carried out under mild reaction conditions in terms of pressure, temperature and pH.

In the past hundred years, a multitude of industrial biotechnological processes have been developed whose efficiency exceeds that of chemical processes, which has helped to establish them in the long run. One of the great challenges of industrial biotechnology is the development of biocatalysts that are active at high substrate and product concentrations that are normally toxic to enzymes and cells. Biocatalysts work almost exclusively in aqueous media; however, the bulk of intermediates and products of fine chemicals demonstrate poor solubility in the aqueous phases; the optimisation of biocatalysts for use in organic medium is therefore necessary.

### Bulk chemicals

Bulk chemical products are products whose production exceeds 10,000 tons annually. Industrial biotechnology will substantially affect the future production of bulk products and polymers. It is expected that an increasing amount of bulk products and polymers produced by chemical means today will be produced by biotechnological processes in the future. High-volume, biotechnologically produced goods are to be found in the food, livestock feed, drinks, detergents, textiles, automotives and energy industries. Examples of products manufactured biotechnologically are given in the table below.

*Table B.1: Bulk products manufactured by biotechnological processes*

| Products | Global Annual Production *(Tons)* | World Market Price *(€/kg)* |
|---|---|---|
| L-Glutamic acid | 1,500,000 | 1.20 |
| Citric acid | 1,000,000 | 0.80 |
| L-Lysine | 1,000,000 | 2.00 |
| Lactic acid | 150,000 | 1.80 |
| Gluconic acid | 100,000 | 1.50 |
| Vitamin C | 80,000 | 8.00 |

Monomers and polymers produced by biotechnological processes for the plastics and other functional polymer industry are becoming increasingly interesting from a commercial point of view. In the past few decades there has been a decline in the number of innovations in the field of oil-based polymers. Biotechnologically produced polymers, such as polylactide (PLA) and polyhydroxyalkanoates (PHA), monomers such as isosorbide and 1,3-propanediol could provide the basis for an innovation impulse.

The development of customised enzymes and the reprogramming of the metabolism of microorganisms open up completely new possibilities for providing biotechnological solutions in the area of basic chemicals and intermediates. Acetone and butanol are examples of products that were manufactured biotechnologically in large quantities in the first half of the 20th century, but are produced today from petroleum. For products such as adipic acid and succinic acid, biotechnological routes exist that could be resorted to if petrochemical raw materials become too expensive or if biotechnological processes provide an additional advantage. This is a promising field of activity for IB in the long term.

## Biofuels and bioenergy

The EU's dependence on energy imports is already 50% and is expected to rise over the coming years if action is not taken, reaching 70% by 2020. This is especially true for oil and gas, which will increasingly come from sources at greater distances from the European Union, often with geopolitical risks attached. Attention will therefore increasingly focus on security of supply. Renewable energy as an indigenous source of energy will have an important role to play in reducing the level of energy imports, with positive implications for balance of trade and security of supply[1].

In the case of road transport, bioethanol and biodiesel are beginning to have a significant impact on the mix of fuels in some countries. Mixed with conventional fuels, they can be used in standard engines without modification, and they also improve combustion and reduce air pollution.

Ethanol (or ethyl alcohol) is produced in far larger quantities than any other fermentation product: 26 million tons in 2002. Nearly two-thirds of this is used as fuel. Brazil leads the world, producing 8.7 million tons of bioethanol for fuel, followed by the USA with 5.7 million tons. The European Union, in contrast, made only 1.6 million tons in the same year, but has recently set itself ambitious new targets[2]: by 2010, 5.75% of both petrol and diesel will comprise biofuels, rising to 20% in 2020.

Ethanol is currently produced from easily fermentable agricultural materials such as sugar cane (in Brazil), sugar beet or cereal grains (in the USA and Europe). But there are vast quantities of waste materials such as straw, corn cobs or even waste paper available, and research is underway to modify microorganisms to use them as an efficient substrate, or to make enzymes, which can cost-effectively break down cellulose to easily-fermentable glucose. Success here would greatly improve the overall economics of ethanol production.

Biodiesel is produced from vegetable oil (typically rapeseed oil in Europe) using a process of chemical modification. Development of a biological process based on lipase enzymes would improve the process efficiency and environmental impact.

Biomass can also be fermented to produce methane (an efficient and established technology) or hydrogen (still in the development stage). Either of these could be a partial replacement for natural gas.

## Fine and specialty chemicals

The term 'fine chemicals' refers to substances that are highly functional and for which world-demand is typically in quantities of less than 10,000 ton per year. From a chemical point of view, these products are usually distinguished by having several functional groups and frequently possess some form of chirality. Classical syntheses of these substances include several reaction steps using stoichiometric quantities of reagents and often deploying extravagant protective group strategies, expensive noble metal/heavy metal catalysts and harsh reaction conditions. Here biocatalysis allows synthesis under considerably milder reaction conditions, e.g. pressure, temperature and pH. A potential application in the pharmaceutical industry is the bioproduction of Advanced Pharmaceutical Ingredients (APIs), which are key building blocks for the synthesis of drug molecules and other chiral molecules.

There is a widespread consensus that a strong impact of industrial biotechnology can be expected in the fine chemicals sector. The current world market share of biotechnological processes in this area is estimated to be some € 50 billion, the potential volume within the next 10-20 years is estimated to be some € 300 billion.

In this respect the crucial factor is time-to-market. In the highly competitive area of fine chemicals this criterion can be decisive. It is therefore not surprising that in the last few years, investments tend to have been made in techniques to accelerate market entry. They include high-throughput screening systems and microsystems for process development.

The simplest case of chiral compounds is one of the two mirror images of a molecule. Chiral compounds are important building blocks for pharmaceuticals, agrochemicals, liquid crystals and other fine chemicals. Chiral compounds can be manufactured industrially in different ways; generally a distinction is made between physical, chemical and biocatalytical methods. A comparison of chemical and enzymatic catalysts shows that in many cases biocatalysts are far superior for the production of chiral compounds due to their higher stereo-, regio- and chemoselectivity.

A recent publication shows that 22 out of 38 large-scale asymmetrical syntheses already apply industrial biotechnology methods[3]. This is only possible because industrial biotechnology can use economically competitive approaches and methods; in the evaluation, sustainability only takes second place, even though it is one of the main driving forces behind industrial biotechnology. At present, due to the excellent enantioselectivity of enzymes, industrial biotechnology methods are primarily used for the production of chiral compounds. Straathof et al. (2002)[4] list 134 industrial biotransformations, of which almost 90% are described as chiral fine chemicals. In the future, this field will undoubtedly acquire greater importance and new reaction sequences for the production of compounds with several stereo centres will be established.

In the area of the food industry, enzymes and whole-cell processes are now widely used in the processing of fruit juice, cheese, wine, edible oils and animal feeds. The production of many sweeteners is now entirely carried out by enzymatic processing based on the conversion of starch; for example, the artificial sweetener aspartame is made from two amino acids produced by fermentation, and erythorbic acid (an antioxidant) is made directly by fermentation. Other amino acids are produced in a similar way on a large scale: in particular glutamic acid, used as a taste enhancer in the form of mono-sodium glutamate, has a production volume of more than one million tons annually, comparable with many important petrochemicals. In the animal feed industry, the amino acid lysine is produced by fermentation, and work is underway to develop a similar process for methionine. Both are used as nutritional supplements in feed.

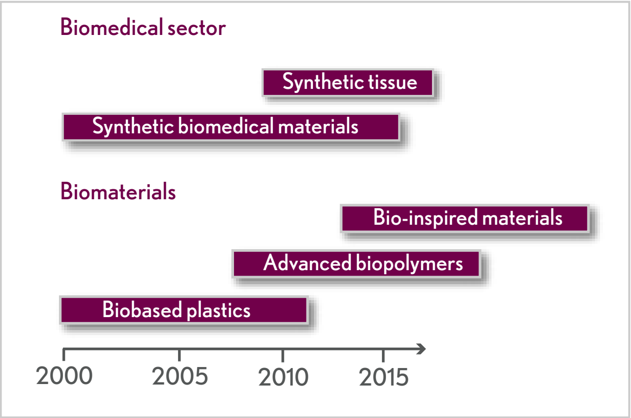
### Bio-based polymers and materials

Two main application fields for 'Biopolymers' can be distinguished, namely the biomedical sector, and conventional and novel polymeric biomaterials. The main focus of this section is on the industrial manufacturing of materials, their monomers and their structuring. On a debatable time scale, several major developments were identified in each sector, as shown schematically in Figure B.1 below.

The **biomedical sector** currently focuses on the development of synthetic materials for medical use (contact lenses, implants, etc.) where biocompatibility plays a dominant role. It is foreseen that in a growing number of applications, malfunctioning original tissue may be replaced by healthy repair tissue supported by a temporary or permanent matrix. Developments in this field are driven by interfacing medicine, molecular and cell biology, as well as mechanical and electronic engineering. Production volumes will be relatively low but the added value high.

Within the **biomaterials sector**, three main developments can be distinguished: bio-based plastics (polymers) based on renewable feedstocks; advanced polymers with more and multiple complex functional properties; and bio-inspired materials where biological systems or production methods have served as an inspiration for a complex structured product.

*Figure B.1: Time line for the development of new bio-based polymers and materials*



### Bio-based plastics

Industrial biotechnology potentially offers novel routes to manufacture chemicals on the basis of renewable feedstocks such as agricultural crops including fibres, co-products and residues (bagasse, husks, etc.). Typical examples are novel monomers for polyesters and similar materials such as lactic acid (LA), 1,3-propanediol (PD), isosorbide and hydroxypropanoic acid (HP) and their (co-)polymerised versions, and potentially existing monomers currently made from petrochemical feedstocks for which biotechnological alternatives are being developed (amides, ethene, acrylic acid, etc.). Biopolymers can be synthesised from bio-based monomers or can be manufactured via functionalisation of natural polymers like chitin, (ligno-)cellulose, gums, proteins and starches. A significant example of a successful application of renewable feedstock is the commercialisation of biodegradable starch-based plastics, which are already produced in a volume of about 75,000 tons per year. The possibility of substituting fossil-based starch-complexing agents with bio-based ones is an important goal to increase the sustainability of biodegradable plastics.

In 2002, Cargill Dow, today NatureWorks, started the biotechnological production of L-lactate in Blair, Nebraska. Lactic acid is used to produce 140,000 tons per year of PLA, a biodegradable plastic. Since 1998, Toyota has used bioplastic components in their Prius and Raum models. A pilot plant for the production of approximately 1,000 tons per year of PLA was completed in Japan in 2004. Toyota plans to cover approximately 66% of world demand for bioplastics by the year 2020 by expanding its own PLA production. The company assumes that by 2020, the bioplastics share of world plastic production will be around 20%. By launching its bioplastics production, Toyota hopes to achieve a turnover of € 33 billion by the year 2020.

### Advanced biopolymers

Biological molecules have rich physico-chemical behaviour, mainly due to the abundance of functional groups at close proximity, which allows for a variety of directional and random interactions. Advanced biopolymeric materials will display new (improved) properties (durability, service life, recyclability, etc.) and will be suitable for an increased number of applications. Although many of the needs are known and expressed by the industry, it is likely that many of these developments will take up to 10 years to reach their full commercial potential (mid/long-term):

- Mono-dispersed oligomers/polymers.
- Chiral oligomers/polymers (for coatings/pigments).
- Liquid crystal character.
- Block-copolymers and other new polymers.
- New building blocks (high T, high-mechanical properties, high-flow).
- Optical clearance and dimensional precision.

### Bio-inspired materials

Scientific and technological developments create new opportunities (application possibilities and needs / new markets). Developments in this area are typically long term (> 10 years). In this case, nature serves as an inspiration for entirely novel structures as well as new manufacturing processes:

- Electronics, e.g. solar cell efficiency needs controlled transport phenomena, attainable through fractal structures.
- Biostructures: protein crystals and inorganic structures (e.g. bones, shells).
- Dimension stability, miniaturised structures and devices.
- Surface structuring on very small scales (e.g. data storage).
- Barrier properties.
- Chemical / physical sensing (e.g. smart packaging, personal identification, etc.).
- Interference colouring / multi thin layer structuring (pearlescence of chitine).

## Bio-based Performance Materials

Bio-based performance and nanocomposite materials are polymeric materials, which are produced by or from microorganisms or other biocatalysts, and which feature specific functionalities based on the micro/nanostructure of the material, derived from self-organisation. Other bio-based performance and nanocomposite materials are the result of the rational design of biomaterials that utilise the principle of natural self-organising materials. There is more and more interest in the preparation of modified surfaces for bioadhesion, biosensing, and drug delivery. Therefore multidisciplinary research is needed, combining elements of organic and polymer synthesis, physical methods, biotechnology and engineering. The combination of proteins and inorganic materials, often with specific nanoscale geometry, offers new and innovative product areas such as self-cleaning, self-repairing and sensing products.

A variety of thin film processes and surface investigation techniques can be applied to new synthetic materials and biotechnology-oriented projects. The development of new polymers using biotechnology is a field of research of enormous potential. Combinations of naturally occurring polymers and biomaterials, as well as synthetic polymers and biomaterials, display a rich variety of complex structural and dynamic behaviour. Other examples are the design of new multi-component materials and network polymers with materials such as chitosan derivatives and polyalkyleneglycols.

New performance biomaterial can be (largely) bio-based or at least bio-inspired, i.e. made of bio-based building blocks, or designed using principles derived from biopolymers, or made by enzymatic modification of biopolymers. New performance biomaterial can contribute to the following applications:

- Controlled release of drugs and nutrients.
- Smart packaging materials.
- Eco-friendly antifouling coatings.
- Smart materials (e.g. membranes, adsorbants) for separations of (bio)molecules.
- Smart surfaces and matrices for the immobilisation of enzymes and receptors.
- Self-cleaning surfaces.
- Self-organising polymers.
- Hard- and software for analysis.
- New biomaterials with properties that were considered 'impossible' in the past.

## Other Bio-based Chemicals

### Sugar-based chemicals

The importance of sugar-based production of chemicals will rise dramatically in the future. Fermentation technology in particular opens the gate to a vast variety of building blocks with carbon chain lengths varying from 2 to 6. This platform technology will lead to intermediates suitable for the polymer industry, the biofuel industry and the pharma industry. Additionally the sugars might be used directly for the production of sugar derivatives as e.g. sugar-based surfactants or sugar-based modified food products. Examples of sugar-based products made by fermentation or potentially accessible with biotechnological tools are:

- Alcohols like e.g. ethanol, butanol, etc.
- C3 building blocks like e.g. glycerol, 3-hydroxypropionaldehyde (3-HPA), 1,3-propanediol (1,3-PDO), lactic acid, malonic acid.
- C4 building blocks like e.g. succinic, malic or fumaric acid.
- C5 building blocks like itaconic or glutamic acid.
- C6 building blocks like sorbitol or gluconic acid.
- Sugar oligomers like e.g. cyclodextrins or chitosan oligomers.
- Sugar-based surfactants / biosurfactants.
- Sugar derivates like sugar esters with fatty acids for cosmetic and food applications.

**Oil / lipid-based chemicals**

Plant oils and animal fats serve as the basic renewable feedstocks for the oleochemical industry to produce fatty acids, methylesters, fatty alcohols, surfactants, all kinds of ester and ether products and glycerol. Chemical processes traditionally drive the oleochemical industry. A lot of products offer the opportunity for the development of an 'alternative' biotechnological process. The continued rise in oil prices could stimulate the search for low temperature biotechnological conversion processes, especially when these can be more economically viable than the traditional high-temperature processes. Biotechnological processes have recently been introduced into the oil and lipid transforming industry, namely enzymatic interesterification and enzymatic degumming of crude oils. Examples where biotechnology could play a role in the future are:

- Enzymatic oil splitting to yield fatty acids and glycerol; this process has been investigated in the past, but could now become an economically viable process.
- Enzymatic production of methylesters (and biodiesel).
- Enzymatic ester synthesis like e.g. emollients or emulsifiers.
- Lipid-based biosurfactants.
- Lipid-based biolubricants.
- Polyol modified lipids for the polymer industry, which might be obtained through biotechnological oxidation reactions.
- Structured and 'Designer' lipids for e.g. food and pharma applications.
- Microbial oils with nutritionally valuable ingredients.
- Utilisation of glycerol as building block.
- Biotechnological utilisation of waste oils.

**Protein-based chemicals**

Proteins may be used in the form of their hydrolysates for nutritional, feed and cosmetic applications. The choice of enzyme used determines the product properties. Furthermore, the amino acids obtained by full hydrolysis are interesting building blocks for the chemical industry. Other substances on the basis of proteins accessible by biotechnology could be amino acid and peptide-based surfactants or polymers obtained through biotechnological cross-linking procedures.

## 2 Research and Development Highlights

**"Oxidoreductase enzymes as industrial biocatalysts for fine and bulk chemistry"**

Regio- and stereo-selective oxidation reactions (e.g. non-activated carbon atom hydroxylations, double bond epoxidations, aromatic hydroxylations, heteroatom and Baeyer-Villiger oxidations) are of paramount importance in organic synthesis, and conventional chemical techniques have not yet been able to solve all the associated problems. The addition of oxygen to inactivated carbon atoms cannot be achieved with traditional synthetic methods, but the use of mono-oxygenases, dioxygenases, and peroxidases is emerging as an alternative to overcome these limitations.

Conversely, less selective oxidations performed by laccases are also of particular industrial interest in the development of new processes to convert lignin into bulk aromatic chemicals and in the development of biosynthetic processes to convert monomers into new functional and hybrid biopolymers, to produce new antimicrobial and anticancer molecules, food additives and environmentally-friendly dyes.

Oxygenases (mono and di) have the necessary versatility and selectivity to cope with many of needs of the chemical industry. In the field of bio-based polymers, sustainable processes to convert fatty acids into dicarboxylic acids (monomers useful for producing biodegradable bio-based polyesters) through ω-oxidation are needed. As another example, the intrinsic stability and flexibility of laccases offers opportunities to achieve radical coupling synthesis. However, for industrial applications some problems still have to be overcome:

a) Effective oxygen supply when whole cells are used (new oxygen spargers, new reactor design and organic-aqueous systems in column air-stirred reactors).
b) Substrate and product inhibition (*in-situ* substrate supply and product removal).
c) Coenzyme recycling (development of a generic coenzyme-recycling expression vector, which will produce novel two-in-one recombinant biocatalysts in which the oxygenase is fused to a coenzyme regenerating counterpart).
d) Substrate versatility and selectivity (toolbox of various recombinant biocatalysts with a large range of selectivity obtained through genomic database mining).
e) Stability of whole cells as well as of isolated biocatalysts (immobilisation entrapment, additives, chemical modification*) .
f) Novel bioreactors, e.g. biofilm reactors, new construction materials and geometries (compact reactors with reduced liquid hold-up).
g) Effective integration of green chemistry, process engineering and bioconversion processes to reach higher productivity and sustainable industrial breakthrough.

There is also potential in the use of biocatalysts for some reduction reactions. There is for example a literature precedent for bioreduction of amides to amines and for the conversion of nitroaromatics to anilines; these opportunities should be seized and brought to fruition. While the reduction of ketones to secondary alcohols using microorganisms has been documented extensively, the technology still requires optimisation. In contrast, the bioreduction of imines to amines is virgin territory. But perhaps the most intriguing area for exploration is the asymmetric reduction of electron-poor alkenes using intact cells rich in enoate reductase. Bakers' yeast partially fulfils the requirements, but a focus on this area should yield catalytic systems that would complement chemical catalysts.

A comparison should be done between the performance of whole-cell and isolated-enzyme systems (and also conventional chemical processes, when applicable). Work on whole-cell systems should address the conditions for obtaining a self-sustaining population through controlled growth on a mineral medium and an appropriate carbon source to ensure required catalytic activity. A cell population with controlled activity and cofactor regeneration capacity is advantageous for continuous processes.

* Points d. and e. should also be tackled by site directed mutagenesis and/or directed evolution (the latter involves the development of suitable High Throughput Screening).

## Biomass conversion to fuels

Biomass already contributes 5% of the EU energy supply, and 65% of total renewable energy production, where it is predominately used for heat and power applications. In order to increase the share of biomass used as an energy source, work dedicated to transport fuels production must also be done. Research must play a key role in overcoming technical as well as non-technical barriers.

The predominant technology for converting biomass to ethanol is fermentation followed by distillation. At present, ethanol production by fermentation uses crops with a high content of easily fermentable carbohydrates (cereals, sugar beet, sweet sorghum, Jerusalem artichoke). Processes essentially include the same steps: preparing and hydrolysing the feedstock, fermenting simple sugars, and recovering the ethanol and residual materials. Current ethanol production from high-carbohydrate crops can be further improved to lower costs, environmental impact, and increase yield.

However, bioethanol will only be competitive with fossil fuels on a large scale if it reaches critical mass and expands its market. If vast amounts of biomass can be used for the production of ethanol fuel, economies of scale could be achieved. This would also contribute significantly to the reduction of greenhouse gas emissions. In addition, the development of dedicated bioenergy crops will help rural development and address the challenges introduced by the Common Agricultural Policies as stated in the White Paper on renewable energies1.

## Production of ethanol and ethanol derivatives from ligno-cellulosic biomass

### Biomass feedstock collection*

A large variety of biomass feedstocks are currently available for producing ethanol in Europe. Biomass feedstock would primarily be sourced either as waste products from agriculture (straw), forestry (thinning wood, residuals) or wood-based industries (sawdust, 'black liquor' from pulp and paper industry) or as energy plants specifically grown for the purpose (short rotation trees or other cellulosic material)[5]. Sustainable technologies need to be developed in the EU to be capable of supplying ligno-cellulosic biomass to the future bioenergy industry. Advances in feedstock production will have crosscutting impacts on the conversion of biomass to fuels and chemicals. To develop biorefineries based on agricultural residues, certain barriers must be overcome: security of supply, physical and chemical composition variability, sustainability of biomass removal, feedstock collection, transportation and handling.

### Biomass conversion by hydrolysis

Biomass hydrolysis technology involves the breakdown of biomass into its component sugars by a range of chemical and/or biological processes. Biomass is first subjected to pre-treatment to hydrolyse the hemicelluloses and expose the cellulose for subsequent enzymatic degradation, a process that produces an intermediate pentose (C5) sugar stream. The cellulose then undergoes enzymatic hydrolysis to produce glucose, which can be converted to biofuels and chemicals by fermentation. Residues can be separated and used for power generation for this or other processes.

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* Biomass collection and technical barriers link with biomass availability and quality will be considered by the Technology Platform on Biofuels and by the Technology Platform "Plants for the Future".

The development of various hydrolysis techniques has gained major attention over the past 8 years or so, particularly in Sweden and the US. However, cheap and efficient hydrolysis processes are still not available and some fundamental issues need to be resolved through further development. To develop the capability for biomass conversion by hydrolysis, rigorous R&D needs to be conducted to overcome technical barriers, especially on biomass pre-treatment and enzymatic hydrolysis. Supported by the EU, testing and demonstration of the technology, when developed, will advance the commercialisation of biomass conversion dramatically at both pilot- and demonstration-scale. Scalability, environmental impact and cost of the biochemical conversion processes will all need to be evaluated.

The key technical barriers to the biomass hydrolysis technology exist in both processing and conversion, ranging from insufficient knowledge of the fundamental chemistry to technological deficiencies in reactor and equipment design:

- Cost-effective pre-treatment of biomass to open the structure and allow efficient enzyme hydrolysis of the cellulose. This will require better understanding of pre-treatment technologies, as well as new, more reliable reactor and equipment design.
- Lack of cost-effective enzymes: New generations of cheap enzymes for hydrolysis of cellulose to glucose need to be developed on the R&D frontier.
- Reduction of inhibitory substances in sugar streams: There is a need to develop methods that do not lead to the formation of inhibitory substances or alternatively permit their economic removal so that the fermentation afterwards is not inhibited.
- Co-product development: Fermentation residues are usually burnt to recover the heat and generate electricity. Other approaches can be more cost-efficient: lignin can be extracted as a co-product for other purposes, and other residues with increased protein content can be used as animal feed.

**Fermentation to bioethanol through new and robust microorganisms**

Once the ligno-cellulosic biomass feedstock has been hydrolysed into a mixture of carbohydrates (typically glucose and pentose sugars), these must be fermented into ethanol. The microorganisms used must be able to fully convert the carbohydrates into ethanol, be robust, and tolerant of the toxic compounds formed during the pre-treatment process. They must be able to withstand the stress of high ethanol and substrate concentrations, low pH, etc. At present, no such strains are available, and significant challenges still lie ahead to develop such robust production microorganisms. Developing such strains requires a multidisciplinary approach involving various aspects and research areas:

- Metabolic engineering of metabolic pathways to expand the substrate usage spectrum of the microorganism, possibly involving new pathways and enzymes.
- Identification of microbial stress response mechanisms and subsequent engineering of the system into the production microorganism.
- Engineering high ethanol tolerance into the production microorganism.
- Engineering fast growth, high ethanol yield and productivity into the production microorganism.
- Engineering microorganisms that produce the required hydrolytic enzymes to complete the hydrolysis of biomass during the fermentation process.

## Bio-based performance materials and nanocomposite materials

Bio-based performance and nanocomposite materials are mostly polymeric materials which are produced by or from microorganisms or other biocatalysts, and which have specific functionality based on the micro/nanostructure of the material (derived from self-organisation). This term is also applied to materials 'inspired by nature', which are the result of rational design of biomaterials using the principle of natural self-organising materials.

The development of new polymers using biotechnology is a field of research of enormous potential. Combinations of naturally occurring polymers and biomaterials, as well as synthetic polymers and biomaterials, display a rich variety of complex structural and dynamic behaviour. Combinations of proteins and inorganic materials, often with specific nanoscale geometry, offer new and innovative product areas such as self-cleaning, self-repairing and sensing products. Other examples are the design of new multicomponent materials and network polymers with materials such as chitosan derivatives and polyalkylene-glycols.

In order to produce materials with the required properties described above, extensive research on both basic and applied subjects is needed. Concerning basic research, studies should be devoted to:

- The basis of molecular assembly in living systems.
  The biological cell functions because of self-organisation, but what is the molecular mechanism for this?
  For instance, what is the exact nature of the interactions between proteins and membranes? This should lead to molecular understanding at such a level that accurate predictions could be made concerning the manner of self-assembly of biomolecules, and the magnitude of their interactions.
- The basis of molecular recognition in living systems. If we understand how nature's receptors function, we can design and produce them ourselves and use them to make advanced sensors, for instance for the prevention and timely detection of serious diseases, the detection of toxic agents and biohazards at low concentrations, etc.

Using the knowledge obtained in the basic studies, it should be possible to develop new materials for the applications below. These materials should be (largely) bio-based or at least bio-inspired. This means that they are constructed from bio-based building blocks, designed using principles derived from biopolymers, or made by enzymatic modification of biopolymers.

- Controlled release of drugs and nutrients.
- Smart packaging materials.
- Eco-friendly antifouling coatings.
- Smart materials (e.g. membranes, adsorbants) for separations of (bio)molecules.
- Smart surfaces and matrices for the immobilisation of enzymes and receptors.
- Self-cleaning surfaces.
- Self-organising polymers.
- Hard- and software for analysis.
- New biomaterials with properties that were considered 'impossible' in the past.

# 3 Demonstration Project: "An Integrated and Diversified Biorefinery"

## General description

This demonstration project has the potential to be trendsetting, opening new perspectives and, most importantly, crossing borders in both a technological and industrial as well as geographic sense. While building on existing European knowledge and capacities, it should aim to explore and develop new R&D sectors as well as prototyping and introducing new technologies for future industrial applications. An important aspect of demonstration projects is to study and show societal, environmental and economic benefits of a new technology – in this case industrial biotechnology - implementing therefore the three pillars of sustainability: People, Planet and Profit.

To be successful, R&D funding is needed together with broader support to set up innovative pilot plant(s). Funding will be sought through a Public-Private Partnership involving industry, academia and research institutes, the European Commission, the European Investment Bank and Member States.

An integrated and diversified biorefinery is an overall concept of a processing plant where biomass feedstocks are extracted and converted into a spectrum of valuable products. Biorefineries combine and integrate necessary technologies from the biomass supply and conversion technologies through the core bioprocessing and downstream processing steps towards the final application of use for society, covering therefore the whole industrial biotechnology value chain.

The project will develop different technologies to convert biomass raw materials into industrial intermediates and consumer products. These will be a small number of specific bio-based target products and applications in each of the categories of fine and speciality chemicals, bulk chemicals, biofuels, bio-based polymers and performance materials. The best candidates will be identified through a call for projects, according to the quality of the proposal, the balance of realism versus technological ambition, the innovation potential and the final use of the product.

The products of such an integrated biorefinery should typically be highly diversified, for example:

- The production of 2nd generation biofuels.
- The development and production of (new) platform chemicals for bulk products.
- The development and production of (new) biospecialities.
- The development and production of (new) bio-based performance materials.

Biomass feedstocks have so far mostly been studied for the production of biofuels and energy, and less has been done on transformation of biofeedstocks into chemicals or materials. However, the total size of the European polymer market today is 3 million tons per year. This is considered the most important field for developing the use of renewable raw materials. Polymers are the largest non-energy application area for fossil feedstocks and will provide the largest number of potential applications from renewable resources. Most of the projects carried out to date have focused either on biopolymers or biofibres but not on biocomposite materials.

## Project work packages and deployment

To develop the concept of biorefinery based on renewable biomass raw material, the main objectives of research are:

- Development of complex systems of sustainable technologies.
- Development of new materials and new manufacturing technologies.

Technological development will focus on:

- Development and/or selection of raw material for specific applications.
- Development of new procedures of enzymatic or chemical modification of biomass and transformation to monomers.
- Development of new technologies for polymerisation, fibre pre-treatment and polymer processing.
- Development of cost-effective, environmentally-friendly biodegradable biomaterials and biocomposite materials and products made from them.

**Biomass supply and conversion**

Amongst biofeedstocks, cellulose and lignin are the most abundant renewable resources on Earth. However, their efficient utilisation in isolated form has not yet been successfully achieved. The main reason is that their macromolecules are too heterogeneous and complex. For the biomass supply and conversion technology, a phased deployment strategy will be used in the project.

Phase 1: The starting material will be starch, a readily available carbohydrate source from current biorefineries that can be easily converted into glucose.

Phase 2: The future biorefineries should necessarily process the whole crop to be economically competitive. Phase 2 will deal with increasingly difficult biomass sources such as cellulose, ligno-cellulosics and ultimately crude biomass and organic waste.

The first challenge is the efficient separation of the three main components: the cellulose, the lignin and the hemicelluloses. Today, enzymatic hydrolysis of the cellulosic portion of ligno-cellulosic feedstock to glucose and cellobiose is a versatile and flexible means of utilising ligno-cellulosic biomass, though not yet economically feasible.

The second challenge is adding value to the separation and conversion products. The glucose, cellobiose and xylose produced can either be used directly in the food and biotechnology industry, or used as a platform for producing a variety of bulk and speciality chemicals, including fermentation to ethanol. Economically useful applications for the lignin remain a great challenge, despite numerous research efforts. What quality of lignin should we aim for, for what application? Biofuels are one of the main outlets, but interest must also be directed towards some intermediate components for chemical applications or towards high value-added molecules.

The third challenge is to define the optimal biomass according to its availability and the nature of the final application. By way of example, bulk applications such as biofuels will obviously be directed towards the use of ligno-cellulosics as the ultimate biomass source, whereas food applications will tend to use glucose as a pure and convenient food-grade raw material.

**Bioprocessing**

The technological focus will be on improving processes based on standardised feedstock, and developing new processes for the production of novel biochemicals and biomaterials.

Several sub-projects will need to tackle the various technologies that are required to convert the carbohydrates into the target product: enzyme production and biocatalysis, metabolic engineering in all its aspects, bioprocess integration and new downstream processing techniques such as *in-situ* product recovery. Microbial stress will need to be addressed to overcome the inhibitory effects of the product that typically reduce the overall yield and efficiency of the process. The main challenges associated with bioprocesses are described in detail in the *Reaction and Process Design* section.

### Innovative bioproducts

If the product target is a new compound, research towards the development of applications for the compound will also be included in the demonstration project. This technological development can include e.g. for the production of bioplastics:

- Chemical technologies for the polymerisation of biomonomers into bioplastics.
- Development of new technologies for fibre pre-treatment and polymer processing.
- Application research on possible uses of the produced bioplastics.
- Biodegradability studies in the case of biodegradable polymers.

Bio-based polymers are considered a very important field of industrial biotechnology application, in terms of bringing volume to the market. Polymers are the largest non-energy application area for fossil feedstocks. Moreover, cost-effective, environmentally-friendly and biodegradable bioplastics are an expanding field with interesting applications. Furthermore, the current high price of petroleum provides strong incentives for the development of bioplastics.

Well-known examples of industrial biotechnology products are fermentation products such as antibiotics, amino acids, vitamins and enzymes, products related to medical, food and feed applications. Most amino acids are now exclusively produced through industrial biotechnology in large-scale industrial processes. In other cases, like the water soluble vitamin B2, biotechnological processes successfully replaced chemical productions, due to lower costs and improved eco-efficiency.

In contrast, most industrial chemicals and polymers are still produced by chemical synthesis from oil and gas. Recently however, new pilot and production processes for biopolymers like PHA or biomonomers like 1,3-propanediol, isosorbide or lactic acid have been announced by a number of companies. The production of solvents such as ethanol, isopropanol, butanol and acetone from ligno-cellulosic materials as an integrated process would also be of interest.

Other high-value products must be considered as co-products of the integrated and diversified biorefinery in order to make it economically interesting and sustainable, for example biospecialities, bio-based performance and nanocomposite materials.

### Benefits and added-value of the technology

A further important aspect of the demonstration project is to study and show societal, environmental and economic benefits of the new technology, according to the three pillars of sustainability: People, Planet and Profit. Lifecycle assessment studies, impact assessment and eco-efficiency studies must be integrated in the demonstration project in order to demonstrate the benefits of the new technology.

## 4 Accompanying Actions and Issues

The SRA needs to be supplemented by an action plan based on the following principles:

- **Long-term planning and continuity of research funding**: If industrial biotechnology is to fulfil its promised contribution to Europe's future global competitiveness and industrial sustainability, the commitment to underpinning R&D must be long-term and guaranteed. Scientific expertise has to be built up and nurtured; it cannot be turned on and off at will. Far greater emphasis on industrial biotechnology in the seventh and subsequent Framework Programmes, in line with similar commitments by European trading partners, is therefore essential. In this aspect, the recent FP7 proposal of the Commission, with 'the knowledge-based bioeconomy' as one of the themes, is very promising.
- **Coordination of European and national objectives and policies:** Too much research is currently carried out in an uncoordinated way by the Member States. To achieve the maximum return on research funds and not duplicate efforts, national industrial biotechnology programmes must be run as part of the overarching European research agenda.
- **Promote interdisciplinary cooperation and overcome fragmentation:** Given the multidisciplinary nature of industrial biotechnology R&D, it is vital that the various activities are not left as isolated research 'islands'. Bringing together groups of chemists, biotechnologists, engineers etc. into clusters will provide critical mass, allow them to share support facilities and encourage cooperation and synergy. Such clusters can then, over time, grow into global centres of excellence.
- **Facilitate technology transfer:** High-quality research is of little value if it does not contribute towards innovation and economic growth. All possible steps should be taken to facilitate good working partnerships between universities and industry, including the setting up of public-private partnerships.
- **Focus on overcoming bottlenecks in the technology:** Despite rapid progress in some areas, exploitation of new technologies can often be delayed by bottlenecks in a few key areas. Good overall coordination of the programmes should allow early identification of these problem areas and permit the focus of expertise into concentrated, ambitious projects in order to remove the bottlenecks.
- **Contribution to standards:** High-quality products can differentiate the European products and processes and increase competitiveness of agriculture and industry. Specific standards are needed to identify, qualify and protect high-quality products with the aid of the European standardisation body (CEN).
- **Impact analysis:** To implement industrial biotech goals for sustainable development, it is important to integrate the three pillars of sustainability (People, Planet, Profit) into projects and actions, whenever relevant. The use of instruments such as Lifecycle Assessment (LCA) or Risks / Benefits analysis should be implemented in relevant projects and technology areas. In this context, LCA is intended as a 'steering tool' rather than just as an analytical tool, with the purpose of defining the factors and their relative environmental impact to be taken into account in the whole industrial chain (from agriculture to final waste disposal). It will be equally important to assess the economic impact of industrial biotechnology products as a function of fossil fuel prices, renewable raw material prices and other factors (current situation and prospective economic assessment) as well as to compare their cost- and eco-efficiency with similar existing products.
- **Perception, awareness and education:** One cannot assume that the average citizen will necessarily be comfortable with widespread use of biological processes by industry, particularly in instances where genetically modified microorganisms are used (although in contained environments). In order to assure society's consent, society must be involved in an open dialogue at an early stage. Education is an important factor. It is desirable that future generations should be increasingly scientifically literate, as science forms the basis for sophisticated modern societies to function. Both teachers and students should be encouraged to become more familiar with basic science in general and with biotechnology in particular. Awareness and knowledge about sustainable / eco-friendly products can also be promoted by making information available in brochures and through other channels, and by encouraging visits to factories operating biological processes. But education is by no means the entire answer. Increasing familiarity does not automatically result in increasing acceptance. Dialogue should be established by as many means as possible.

# Materials Technology

***Definition of material science:*** *Generating new knowledge on high-performance materials for new products and processes; knowledge-based materials with tailored properties; more reliable design and simulation; higher complexity; environmental compatibility and environment preservation; integration of nanomolecular macro levels in the chemical technology and materials processing industries; new nanomaterials, biomaterials and hybrid materials, including design and control of their processing.*

## 1 Introduction

The *Materials Technology* section of the *Technology Platform Sustainable Chemistry* is a network of stakeholders from academia, non-profit research institutes, chemical and downstream industry providing an industry driven strategic research agenda for the 7th Framework Programme and beyond.

The discovery of new materials with tailored properties, and the ability to process them are the rate-limiting steps in new business development in many industries. The demands of tomorrow's technology translate directly into increasingly stringent demands on the chemicals and materials involved, e.g. their intrinsic properties, costs, processing and fabrication, benign health and environmental attributes and recyclability with focus on eco-efficiency.

Materials science deals with the design and manufacture of materials, an area in which chemistry plays the central role; there is also considerable overlap with the fields of chemical engineering, biotechnology and physics. Substantial contributions include: modern plastics, paints, textiles and electronic materials; but there are greater opportunities and challenges for the future.

The focus of the *Materials Technology* section is to reflect the views of the European chemical industry, academia and society within the framework of sustainable chemistry by building networks connecting all relevant stakeholders (industry, small and medium sized enterprises, NGOs and academia) in the field of materials technology.

### The tasks of materials technology

The task is to provide guidelines for realising the goals and challenges set by the EU to address the societal needs of energy, healthcare, information and communications technology (ICT), quality of life, citizen protection and transportation (mobility). Five research areas were identified which are discussed in further detail in this chapter: a) fundamental understanding of structure property relationship, b) computational material sciences, c) development of analytical techniques, d) new production processes for the scale-up of laboratory synthesis for improved materials, and e) bio-based performance and nanocomposite materials. The chapter is concluded with a special focus section on nanotechnologies and nanosciences.

## 2 Fundamental Understanding of Structure Property Relationship

### Modelling of synthesis and chemical reactions

**Polymers, copolymers and polymerisation processes**
Over the last decade, molecular modelling has become an invaluable tool for the calculation of material properties based on their chemical constitution, and for the development of novel materials with prescribed properties for a given application. Modelling of synthesis and processing routes can be a powerful tool for determining which course to pursue and which are unfeasible and/or uneconomic. The 'hot topics' in molecular modelling to date are related to the development of innovative synthetic strategies in polymer chemistry, and to the development of environmentally-friendly chemical technologies based on novel solvents (supercritical and ionic-liquid solvent technologies). Detailed understanding of new mechanisms of polymerisation e.g. in catalytic, enzymatic and free radical polymerisation in dispersed media (emulsions, mini-emulsions, etc.) and under supercritical conditions are among these. Purification of solvents remains one of the key problems of sustainable chemistry that still needs to be solved.

Copolymers have been studied extensively for several decades, partly because of their biological and industrial importance, and partly because of their interesting and sometimes perplexing properties. Although recent years have witnessed an impressive confluence of experiments and analytic theories, presently there is no comprehensive understanding of what role copolymer sequences play in the structural and functional features of copolymer systems. For this problem, numerical simulations in conjunction with simple models and theoretical approaches should provide a detailed answer. The simulation methods as applied to design non-trivial sequences in synthetic copolymers, should be aimed at achieving the desired functional properties of the resulting copolymer. In this area, the focus could be on a recently developed computer-aided approach, called conformation-dependent sequence design (CDSD), which takes into account a strong coupling between the conformation and primary structures of copolymers during their synthesis. Ideologically, this approach is similar to that used in the context of protein physics, but it aims at synthetic copolymers rather than biopolymers.

It has been found that conventional synthetic methodologies (polymer-analogous reactions and normal radical copolymerisation) based on CDSD can lead to non-trivial chemical sequences with long-range correlations and to various new functional copolymers including bio-inspired water-soluble amphiphilic copolymers, molecular dispensers, adsorption-tuned copolymers, and copolymers capable of recognising patterned surfaces.

Future work should aim to develop new synthetic strategies following this line, and a set of integrated computational tools to predict the relationships among chemistry, microstructure and material properties of designed copolymers. Hybrid electronic structure/molecular dynamics methods scalable to very large systems are needed to model combined reaction and structure evolution. Computer-aided evolutionary techniques can open the door to the design and synthesis of new biomimetic polymer materials.

Another perspective direction in polymer chemistry is related to molecular modelling of interface copolymerisation at liquid-liquid interfaces and emulsion polymerisation leading to new, commercially viable polymeric materials. Since many polymerisation and self-assembly processes take place in solution, electronic structure simulation methods implicitly or explicitly incorporating solvation are necessary. Further effort has to be made to develop the sol-gel processes for hybrid organic/inorganic materials, which offer soft conditions for the synthesis of innovative materials, especially nanomaterials and coatings.

### Novel solvents

Supercritical solvents, especially carbon dioxide, offer novel synthetic options due to their unusual solvating properties, coupled with the ease of removal and options for phase transfer catalysis. Supercritical fluid chemistry can be used to prepare new materials and nanomaterials such as oxides, nitrides, metals with controlled shape and size, continuously from micronic to nanoscales. Greater emphasis needs to be placed on the fundamental understanding of the structural and thermodynamic properties of supercritical solvents. Particular attention should be given to understand the behaviour of solutions of organic/polymer species in supercritical solvents, from the atomic/nanolevel via microstructure to macrostructure levels using advanced analytical techniques and large-scale computer modelling. Ionic liquids have been described as green solvents, as a result of their low vapour pressure. Ionic liquids are environmentally-friendly reaction media (as compared to the traditional organic solvents), and at the same time, they can provide increased reaction rates, lower reaction temperatures and higher selectivities. They are good solvents for a wide range of both inorganic and organic species so that unusual combinations of reagents can be brought into the same phase. Ionic liquids are non-volatile, hence they may be used in high-vacuum systems and many containment problems are eliminated. Ionic liquids are immiscible with a number of organic solvents thereby providing a non-aqueous, polar alternative for two phase systems; this can be used to affect total catalyst recovery in a number of transition metal catalysed reactions. Recently, some commercial processes have been developed using ionic liquids. The wide variety of ionic liquids available and the possibility of having a tailored synthesis of ionic liquid for given applications, e.g. new conducting materials, opens a great deal of opportunities. However, a lot of research has yet to be carried out before ionic liquids could be used widely in the chemical industry. The separation of the final product from the solvent is a problem that still needs solving; fundamental studies on the properties of ionic liquids and the kinetics and reaction parameters in ionic liquids are still unknown. The use of polymerisable ionic liquids as a gelling medium allows for the fabrication of many new materials. Since ionic liquids are non-volatile, the materials based on them do not shrivel, even at high temperatures and under vacuum.

Despite large number of publications on ionic liquids in the years 2003 and 2004, only a few ionic liquids were studied using computer simulations. There is a wide range of yet-to-be understood phenomena and structures: low interfacial tension of ionic liquids, their stabilising role in microemulsions, and liquid-liquid phase transitions. In view of this, extensive molecular simulation work should be performed, including on the following problems and systems:

- Development of an appropriate atomistic potential model, and force-fields, for modelling ionic liquids.
- Quantitative descriptions of the bulk structure and thermodynamic of ionic liquids, their interfacial properties, reaction kinetics in ionic liquids, and selectivity towards particular chemical and biological agents.
- Liquid-liquid and liquid-solid phase transitions in ionic liquids.
- Interfaces of ionic liquids for applications involving heterogeneous catalysis.
- Mixed ionic liquids where one of the ionic components comprises a dissociating polymer (linear chains, gel-like frame, etc.).
- Emulsification and emulsion polymerisation in ionic liquids.

### Production process

In many cases, the focus of chemical research does not lie on the search for novel structures, but on the optimisation of production processes for basic chemicals, intermediates and fine chemicals.

Computational methods and atomistic modelling have a great potential to optimise the synthesis conditions and structures of poly-electrolytes, ion-conducting polymers and electrochemically active polymer membranes, allowing for maximal conductivity (ion or electronic), and good mechanical strength to enable their use in polymer membranes for electrochemical cells and fuel cells, and in controlled release membranes. Both experimental and computational methods should be used in establishing the structure-properties relationships for such complex polymer systems. A hierarchical modelling approach (combined molecular, mesoscopic and macroscopic modelling) can provide guidance and permit reduction of the experimental work required. This is very important for optimum product and process design. QSAR/QSPR (quantitative structure-activity / property relationships) approaches can also be considered as universal and useful techniques for the modelling and prediction of many properties of chemical compounds and many properties of materials.

## Modelling of catalysis

### Heterogeneous catalysts

Organic, inorganic or metallic catalysts catalyse many important synthetic, industrial and biochemical transformations. Catalytic methods for the transformation of complex molecules are of special importance in the production of fine chemicals. The synthesis and immobilisation of catalytic reactive centres in solid state surfaces, the development of new materials by novel paradigms derived from nanotechnology to provide materials with higher specific surfaces, selective hydrogenation and oxidation, biocatalysis (overlapping with industrial biotechnology initiative) as well as multisite/ multireaction catalysis are of great interest.

Catalysts account for billions of euros in annual business revenues in the European industry. This means that even small improvements in catalyst performance can result in significant increases in profits.

Progress in this area is strongly driven by catalyst design, including the rational design and synthesis of nanoparticle-based catalysts with high activity, selectivity and controllable electronic properties. By tuning the size, composition and shape of the nanoparticle, the surface chemistry, and therefore the catalytic properties of a nanoparticle can be controlled.

For a long time, the search for new and improved catalysts was characterised mostly by the use of empirical, trial-and-error methods. Currently, simulation methods at the atomic and molecular levels are used for virtual screening before more costly experimental activities are pursued. Heterogeneous catalysis has been a focus for simulation effort, with numerous studies of zeolites and metal oxides. But this is an area in which the possibilities offered by new quantum mechanics techniques and molecular simulation methods are particularly exciting, allowing users to study larger, metal-containing, organo-metallic and bio-inspired catalytic systems at a previously impossible accuracy, to simulate the chemical reactions being catalysed. Although heterogeneous catalysis is of enormous industrial significance, the precise processes taking place still remain largely unexplained on the atomic scale for most reactions.

Experimental characterisation of active sites is challenging, and it is rarely possible to perform discrete, systematic adjustments of the active site to probe the influence of discrete variations on performance. Simulation allows specific questions to be asked and can focus costly experimental work on solving particular problems.

One strategic research area is to construct novel, nanoparticle-based catalysts and self-assembled metal-organic complexes with non-covalent bonds for catalytic applications, and to study the structural and electronic properties of these supramolecular systems. Supramolecular nanoparticles containing different noble or transition metals have been found to catalyse a wide range of reactions: hydrogenation, hydrosilylation, hydrogenolysis, Heck-type coupling, oxidation reactions, and direct conversion in fuel cells. Besides the key role of the metal centre, another reason for the high activity and selectivity of nanosized particles is that a large percentage of a nanoparticles metal atom lies close to the surface. These nanoparticles have many other potential applications, including nanophase materials such as quantum dots and nanowires, chemical sensors, light-emitting diodes and magnetised liquids. It will be an integral part of the research, using high-performance computing, to explore new theoretical approaches for catalyst preparation, the modelling of polymerisation catalysts and to gain further insight on the molecular mechanisms of heterogeneous catalysis and on catalyst activation/deactivation at the nanoscale. The complete 'chain of knowledge' should be present: from fundamental catalyst research to applied research for materials.

Research tasks: The work should involve the elucidation of the growth mechanism of metallic nanoclusters, factors governing the growth rate, the formation of metal-containing micelles of block copolymers through reduction of metal salts and the possibility of transferring the nanostructures to other media. In particular, the following topics should be considered:

- Polymer nanostructures as nanoreactors for metal nanoparticle formation.
- Reduction of metal salts in the core of block copolymer micelles, in the highly cross-linked polymer networks, and in the ultra-thin layer of polyelectrolytes deposited onto metal oxides (e.g. $Al_2O_3$).
- Incorporation of catalytic centres into nanofilaments and carbon nanotubes (fibre surface modification, patterning techniques, and templated self-assembly).
- Construction and control of core-shell polymer-based catalytic materials.
- Development of polymer-stabilised bimetallic nanocatalysts.

**Mini-reactors**

These areas of research offer great promise, but will require new theories (approximation models) and computationally intensive studies (see *Computational Material Science*). Theoretical techniques such as state-of-the-art computational methodologies on electronic structure, quantum molecular dynamics simulation, together with mesoscopic continuum methods should be applied to nanoscale catalytic materials. More fundamental understanding of catalysis mechanisms and tools for increasing R&D efficiency are essential.

A promising way to control and accelerate a conventional chemical reaction is to assemble the reagents in a set of microreactors distributed uniformly in the system. To concentrate reagents in limited volume, different heterogeneous systems can be used, such as polymer gels having catalytic sites attached to gel chains, structured polymer gels, dendrimers, micellar and emulsion solutions.

When reagents are amphiphilic (surface-active) compounds, they are preferentially adsorbed at the surface of the emulsion microdroplets, rather than dissolved in either the outer phase or inside the droplets. As a result of such a redistribution of reagents, the reaction rate can increase a hundred fold. Microscopic and mesoscopic modelling of the corresponding phenomena and systems is a very important problem, which can be directly related to biocatalytic process design and the optimisation of industrial biotechnology processes.

**Fuel cells**

Simulation techniques should also be used in a number of aspects of fuel cell research, including development of improved and nanosized catalysts, understanding of membrane microstructure and trans-membrane proton transport. Fuel cells involve the catalysed conversion of a fuel, such as methanol, to carbon dioxide and water. The use of these nanocatalysts will provide the most 'bang for the buck' - higher power density for the same amount of catalyst and, therefore, lower cost for each fuel cell.

**Summary**

By its very nature, catalyst design involves multiple length and time scales as well as the combination of types of materials and molecules that have been traditionally studied in separate sub-disciplines. This means that fundamental methods that were developed in separate contexts will have to be combined, and new ones invented. This is the key reason why an alliance of investigators in catalyst design with those in computer science will be necessary for the success of theory, modelling, and simulation in the field. Because each catalyst research problem is unique, a broad suite of methods is needed. First principles-based and rare-event simulation methods will be essential in describing a number of phenomena, such as the nucleation and growth of metallic clusters, their surface morphologies and diffusion. Density functional theory provides a computationally attractive method for studying conceptual questions in catalysis.

## Modelling of advanced materials and composites

Steels and other metallic alloys, super alloys, carbon materials, polymers, optical, electronic and magnetic materials, superconductors, technical ceramics, composites and biomaterials, hybrid organic/inorganic materials are considered as advanced materials. Nanometric and mesoscopic materials (like fullerenes, nanotubes, and colloids); nanoporous structures (like composite polymers, clathrates) will continue to display surprising properties (optical, mechanical, electric, magnetic, and surface). Smart materials are designed to respond to external stimuli, adapting to their environment in order to boost performance, extend their lifetime, save energy, or simply adjust conditions to be more comfortable for human beings. Materials will be developed that are self-replicating, self-repairing (or self-destroying) as required.

In order to successfully introduce innovations based on new advanced materials into the market, there is a need to control the synthesis and processing. An understanding of the role and interplay between composition, microstructure and performance is necessary. The specific properties of materials, and thus their performance, are largely determined, not only by their composition, but to a large extent by their meso- or microstructure. Morphology, for example, is important for the performance of technical polymers as well as for the rheology of colloidal systems (shampoos). Understanding and the control of phase transformations in general is a prerequisite for optimising the microstructure and hence the performance. Many of these advanced materials will exploit 'nanoeffects'. From the simulation point of view, the nanodomain is particularly difficult. It is dominated by the finite size effects which are close to the quantum regime, but for a purely quantum mechanical treatment, the systems are too large and/or too slow. Atomistic approaches on the other hand, have problems in treating electronic effects. Many of the properties are related to dynamical effects, but dynamics are slow at an atomistic level. Exchange and/or transport of charges (e.g. ion transport in membranes) require a proper treatment of coarse-grained charges to cover the dynamics – something that is currently lacking.

Chemical accuracy still is difficult to obtain for any coarse-graining scheme. It will thus be important to develop schemes that allow bridging from the quantum scale to the mesoscale – with chemical significance and accuracy.

Composite materials, either based on a polymer matrix, on a metal matrix, or reinforced by fibres, have a high potential to lead to new materials with an extremely favourable ratio between strength and weight. Potentially they also offer an advantage in cost-performance ratio, since cheap fillers can be used. These materials can be produced, but their properties and processing still need a lot of attention. A true understanding of the mechanical properties is only slowly emerging, but there is still a long way to go before rational design is possible. The processing problems stem from a lack in fundamental knowledge. The distribution of the filler material in the matrix and the exfoliation process are still not understood in detail. For example, if clay is used as the filler, the processing involves an ionic material that tends to form aggregates. It is unclear how to perform the processing to get a uniform distribution within the matrix. The interfacial properties between particles and matrix, the particles size distribution, and the relevance of the mechanics or transport properties are not understood. Appearance can be modified with additives, as well as chemical stability. How can this all be controlled?

A final point: advanced high-strength/low-weight materials based on composites will not be accepted in construction (e.g. airplane or automotive) industries, unless design procedures are adapted. Lifetime predictions are an issue. In most cases, new materials will require new design. It will be mandatory to have solutions quickly at hand. A truly scale-bridging simulation strategy with appropriate tools will be crucial for market success. Currently, constructors and designers can resort to know-how gathered over decades, when dealing with traditional materials like steel and alloys. In the future, it will be vital for the necessary materials data to be gathered reliably and quickly. A predictive modelling approach must provide materials data for the compounds and the system. Thermodynamic data will be necessary for processing. Estimates of the mechanics will be needed to develop material laws for the finite element modelling of performance, construction and lifetime estimates. These approaches are currently in their infancy. For ideal binary systems, with no direct connections to any particular chemistry, principal insights can be obtained. To make the simulation approaches predictive for 'real systems', it will be necessary to improve these methods.

## Modelling of formulations to achieve controlled functional properties

Formulations play a dominant role in the chemical and pharmaceutical industries. Besides raw chemicals, almost all products are formulated to achieve a certain effect. Obvious examples are adhesives, coatings, laundry formulations, cosmetics etc.; but also nutrition, agrochemicals, and pharmaceuticals rely on formulations to provide controlled release and sufficient stability of the active ingredients.

From a physical-chemical point of view, formulations are complicated multiphase systems, in most cases soft materials. Soft materials are characterised by weak but long-range interactions. Static and dynamic properties largely depend on cooperative interactions on various length and time scales. Most soft materials are based on organic molecules or macromolecules. Colloids consist of weakly interacting nano- or microparticles in a fluid medium. Both inorganic and organic materials are found. In most cases, organic surfactants are necessary to obtain stable or metastable systems. The stability of emulsions and dispersions needs to be improved. Ageing and film formation need to be better controlled. This would have an enormous impact on the coatings and adhesives industries. New processes (e.g. more efficient: continuous reactors instead of batch) could be developed with better stabilised dispersions. So far, finding the right chemistry is more an art than a science. Today, simulations are not really helpful in speeding up the formulation development process, or in assisting in developing improved formulations. With atomistic or coarse-grained molecular dynamics (MD), it is possible to simulate e.g. micelle formation for binary systems. When it comes to 'real' systems (many components, ionic surfactants, salts, impurities), the simulations run into trouble. Principal questions may be answered, but chemical accuracy cannot be expected. There is a need for better simulation methods, because with empirical methods, it will be difficult to improve current formulations. In particular, the proper (in terms of accuracy) treatment of charges on a coarse-grained level is a challenge.

Closely related to this is adhesion. There is a strong need for better control, understanding and improvement of the mechanisms of adhesion, the failure of adhesives, the development of tacky polymers or the prevention of adhesion by surface modification, and better control of the wetting/dewetting process.

Another class of formulated systems are particulate systems, e.g. highly filled polymers, coating formulations, printing inks, etc. Here, the understanding of growth kinetics, surface grafting and modification, polymorphs, etc. is necessary. So far, simulations can give 'snapshots' or ideas what might be going on when a polymer binds to a (generic/ideal) surface. It would be fantastic to be able to design additives with controlled properties for solids, surfaces or formulations by means of computer simulations.
The understanding of physical-chemical processes involved in many formulations mentioned above can be extended to reactive formulations that are of great interest for paints/coatings, adhesives, etc.

## Modelling of interfaces

The main objective of this research is to increase the fundamental understanding of the chemistry occurring at surfaces and interfaces, combining efforts from theory, modelling and simulation through an interdisciplinary approach. The absence of quantitative models that describe newly observed phenomena increasingly limits progress in this field. A clear consensus emerged that without new, robust tools and models for the quantitative description of structure and dynamics of interfaces between liquid (soft) and solid (hard) matter at the nanoscale, the research community would miss important scientific opportunities in nanoscience. The goals should lead to new methods for the characterisation of surfaces and interfaces at atomic and molecular resolution; relationships between structure and composition of the surfaces/interfaces on one hand, and their chemical/physical properties on the other; new materials with pre-designed properties including new heterogeneous catalysts and new colloidal systems; understanding properties of thin liquid films in confined geometry, etc.

## Interfaces: design, characterisation and modelling

Interface engineering is an increasingly important means of improving and optimising many kinds of materials from metals, ceramics and superconductors to bio- and smart materials. This field includes processing and tailoring of surfaces and interfaces for special applications like microelectronics and catalysis. Controlling and manipulating the structure of surfaces on the atomic or molecular scale is a key ingredient for the ultimate miniaturisation of electronic devices, and for the development of new devices that incorporate both solid-state semiconductor structures and molecular materials based on organic or biological components. The long-term impact will be in the development of new molecular electronic devices and of highly miniaturised chemical and biochemical sensors. Simulation methods have been involved in this area from the very beginning and they should play an increasing role during the next few years.

Polymer-surface interactions are of great interest in many fundamental biological processes as well as in various technological applications involving molecular-scale separation processes, controlled surface-induced (template) copolymerisation, immobilisation of proteins, artificial catalysis, phase separation and (nano)structure formation at chemically patterned surfaces, etc. Polymer/solid and polymer/polymer interfaces govern the performance of composites, adhesives, coatings, and incompatible polymer blends. In polymer nanocomposites, where solid nanoscopic particles are added to a polymer, interactions at the polymer/particle nanointerfaces can have profound effects on bulk properties. Specific interactions between a polymer and a solid substrate are important to understand how the polymer can recognise a target surface with a designated pattern. Interfacial molecular recognition is ubiquitous and essential in life processes; examples include enzyme-substrate binding, transmembrane signalling processes, antigen-antibody and protein-receptor interactions. The manipulation of interfaces in these heterogeneous systems at the nanoscale provides a wealth of opportunities to design functional, nanostructured materials for templating, scaffolds for catalysis or tissue growth, and the effect of copolymeric compatibilisers on adhesion.

To develop theories and quantitative understanding of nanointerfaces and interface copolymerisation where surface effects are prevalent and may dominate behaviour at larger scales, it will be necessary to obtain information on the organisation of polymers at interfaces; that is, the arrangement, conformation, and orientation of macromolecules at liquid/liquid, liquid/solid, and solid/solid interfaces. Much of this information may only be accessible by simulation. The geometry and topology of nanointerfaces, bonding at nanointerfaces, structure and dynamics at or near a surface, transport across nanointerfaces, confinement at nanointerfaces, deformation of nanointerfaces, activity and reactivity at nanointerfaces where traditional surface science is generally not applicable, etc. have all to be investigated by simulation. Molecular and nanoscale methods that incorporate phase equilibria and non-equilibrium multiphase systems (including interfaces) are required.

Simulations aimed at understanding the thermal and mechanical properties of nanotubes are very important for applications related to the development of new filled materials whose behaviour is strongly controlled by nanointerfaces.

With further developments in nanotechnology, the need to understand dissipative phenomena, lubrication and friction on an atomic level and in systems confined to the nanoscale increases rapidly.

These studies will ultimately lead to *in-situ* studies of atomic friction on ultra-short time scales. Computational methods have great potential in these areas.

Several grand-challenge problems that will require theoretical and computational advances are identified:

- Interface catalysis and surface nanoreactors.
- Controlled surface-induced (template) copolymerisation leading to various functional copolymers (in particular, copolymers capable of pattern recognising).

## Surfaces: design, characterisation and modelling

Microporous polymer films and coatings represent an important class of materials with applications ranging from ultrafiltration membranes through moisture-breathable plastics to low dielectric constant insulators for semiconductor devices. Highly uniform microporous thin films can be produced from polyelectrolyte multilayers. Due to their high permeability to water, their ability to readily modify the wetability of surfaces, and their ionic nature, polyelectrolyte multilayers are ideally suited as biomaterials. The ability to fabricate microporous thin films from polyelectrolyte multilayers therefore opens up new possibilities for biomedical applications such as cell encapsulation, drug delivery, dialysis membranes, implant coatings, and contact lens coatings.

Currently, research in new biochip technologies focuses on bringing biological function to surfaces. Organic molecules can be induced to self-assemble on glass and silicon surfaces and on microporous gels, allowing for the direct covalent attachment of DNA, enzymes, receptors and antibodies. The ability to pattern surfaces with reactive and inert regions on the nanometer and micron scale allows the generation of high-density arrays of molecules on these surfaces. The corresponding simulation work should be directed towards the construction of microarrays for genomics, proteomics and chemical genetics applications.

New hierarchical materials modelling approaches that span multiple length and time scales, and that couple quantum mechanical methods at the atomic scale to continuum defect modelling at the micron scale, are necessary. Several important problems require computational efforts. In particular, these are the modelling and simulation of:

- Self-assembly of templated nanoporous polymeric materials.
- (Nano)structure formation at chemically patterned surfaces.
- Coating the solid surface with mixed (hydrophobic-hydrophilic) polymer brushes which can change their structure in response to the environment, and are of potential interest for applications such as sensors, switches, microactuators, etc.
- Long-lasting coatings with high scratch resistance and weatherability.
- Smart internal and external coatings with self-cleaning, self-healing and self-repairing properties.
- Surfaces with antifouling properties able to recognise and destroy e.g. pollutants and corrosion agents.
- Functional surfaces with the ability to link reliably biologically active molecules.

All these problems necessitate the use of existing simulation methods, but require that new theoretical approaches and computational tools be developed to provide a fundamental understanding of complexity at the nanoscale, the physics and chemistry of surfaces and nanointerfaces, and how interfaces and complexity at the nanoscale control properties and behaviour at larger scales.

## 3 Computational Material Science

Computational material science tries to provide understanding of materials properties and to assist in the development of new functional materials. It does so by mapping the whole range of technologically relevant processes from chemical synthesis, to experimental characterisation of materials properties to industrial processing onto suitable models and by developing efficient algorithms for their simulation. This encompasses models capturing chemical detail on the scale of individual bonds (scale of about 1 Å) to the scale of the whole molecule, which for macromolecules can reach tens of nanometers. Structures in melts, blends and solutions can range from nanometer scales to microns, millimetres and larger. The corresponding time scales of the dynamic processes relevant for different materials properties span an even wider range, from femtoseconds through milliseconds or even seconds to hours in glassy materials and large-scale ordering processes such as phase separation in blends. No single model or simulation algorithm can span this range of length and time scales. Therefore molecular models for materials range from those including quantum effects and electronic degrees of freedom, to chemically realistic, classical models, to coarse-grained, particle-based 'mesoscale' models that retain only the most essential elements of the material to be simulated, to continuum models that describe the material in terms of, e.g. density or composition variables.

### Bridging of length and time scales in computer modelling

One of the most important problems in computational materials research is multi-scale simulation – the bridging of length and time scales, and the linking of computational methods to predict macroscopic properties and behaviour from fundamental molecular processes. One such step is well-established: going from a quantum-chemically, or density-functionally determined energy surface of a given spatial arrangement of the nuclei making up the material's building blocks to the force-field of a chemically realistic molecular simulation method. Whilst this step is well understood and routinely performed by several expert groups around the world, the next level of mapping, going from a chemically realistic model to a coarse-grained molecular or continuum model, is less well understood. Successful applications of both types of mappings have been reported, but further development on how to combine these levels of description has to be performed in order to create a reliable tool for computational materials science. The next level of mapping from the mesoscale molecular models to continuum descriptions like, for example, those used in finite element methods, proceeds via the determination of constitutive equations for, for example, stresses, dielectric properties or magnetic properties. Linking mesoscale molecular models and continuum descriptions is of paramount importance in the modelling of composite materials, the properties of which are determined by a hierarchy of structures on very different length/time scales. In addition to the mapping between models on different levels of chemical detail, parallel application of different modelling approaches will, of course, remain of great importance. A good example is in the area of organic electronics, where the relevant structural arrangement of the functional units has to be determined by force-field based methods (chemically realistic or even on the mesoscale depending on their size) and the function, i.e. the response of the electronic degrees of freedom can only be described by quantum chemistry.

### Specific interactions

The accurate and efficient modelling of specific interactions is a challenge within computational materials science for two main reasons. The first one is intimately related to the applicability of multi-scale modelling ideas in the presence of specific interactions in the material under study. Going from quantum chemical calculations to a force-field description of a material may have to include short-ranged specific interactions like hydrogen bonds or long-ranged interactions like dipolar or quadrupolar interactions. Specific local interactions like hydrogen bonds lead to local conformational properties, which may no longer be reproducible by a mesoscale model. Whenever these local properties are relevant for the macroscopic behaviour of the material, one may have to resort to an iterative modelling approach alternating between mesoscale and chemically realistic modelling.

The second challenge originates from the long-ranged nature of some of the specific interactions like Coulomb, dipolar or quadrupolar interactions. On the one hand, this is a challenge for the development of efficient simulation algorithms including parallelisation techniques. On the other hand, the correct parameterisation of these interactions may go beyond what can be determined from standard quantum chemistry approaches. Partial charges and local dipole or higher multipole moments can be susceptible to the condensed phase environment of the molecules, that is, to the structural arrangement of the material leading effectively to many body interactions. These are often taken into account by fluctuating charge or dipole models, but at the moment no systematic understanding of these condensed phase effects exist.

Another example of a class of materials where specific interactions are of importance is liquid crystalline materials, where the challenge arises from the presence of anisotropic interactions resulting from the anisotropy of the building blocks. In the ordered state, the molecular anisotropy gives rise to long-range anisotropic strain fields, which in turn may influence the molecules again giving rise to condensed phase effects.

## Development of analytical techniques for materials research via computer modelling

Simulations of physical phenomena provide useful demonstrations that help to develop fundamental understanding and often reveal the essential nature of a process. However, simulations are not just for the classroom, but are essential tools for carrying out modern experiments. To design an experiment, to run it, and to understand the results, a simulation is not an accessory but a necessity. The phenomena under investigation in modern physics and chemistry are usually too subtle, and the experiments too complicated to attack with only analytical tools. Also, the experiments can be too difficult or expensive to perform or can raise environmental or safety issues. Simulations mimic the physical world down to the interactions of individual atoms. These simulations test theories, reveal new physics, guide the set-up of new experiments, and help scientists to understand past experiments. Hence, simulation is essential in the design of modern experiments.

Today, experiment and simulation are more tightly coupled than ever. Indeed, simulations based on quantum mechanics are providing key contributions to the understanding of a rapidly growing body of measurements at the nanoscale. In particular, quantum mechanical simulations provide simultaneous access to numerous physical properties of molecules, such as structural, electronic and vibrational. Furthermore, they allow one to investigate properties that are not yet accessible from experiments or cannot be interpreted explicitly. Standard numerical calculations (e.g. data modelling, data fitting and multivariate curve resolution, factor analysis decompositions of experimental data, expert systems analysis and quantitative structure-activity/property relationships in chemical sciences) are also routinely required to interpret experimental data. Hence, simulations are essential to better understand the physical phenomena involved in experiments. In addition, complex phenomena like those involving industrial processes, where physical parameters cannot be appropriately fixed, are typical examples solved by the traditional model-based data treatments.

Analytical techniques such as high-resolution transmission electron microscopy, scanning probe microscopy, X-ray and neutron diffraction, extended X-ray absorption fine structure (EXAFS), and various kinds of spectroscopy allow the examination of materials at the atomic level. These techniques need to be developed, improved, and extended further by integrating them with more powerful computers for rapid visualisation of data and comparison with computer models. These techniques have a particular importance in the area of materials synthesis, where they can be used for manipulation and control of materials at the atomic and nanolevels, as in atomic force microscopy. The modelling environment that links the simulation methods with advanced analytical techniques can supply a toolkit of common capabilities that permit, for example, the construction of new models, comparison of calculated and observed properties, and iterative adjustment to maximise agreement.

A new and evolving area for simulation technology are real-time applications. In this context the simulation model in conjunction with high-performance computing is used to control a real system. In this case the simulation model can be purposely slowed down to run in real time and to execute in parallel to the real system. During the execution, the model exchanges messages with the controller (the experimental equipment). These messages allow the model and the real system to remain synchronised. These messages are also used by the model to issue commands to the real system to initiate specific tasks. A simulation-based control system has a number of important advantages over traditional control systems. One very important advantage is that a simulation-based control system can, at any point in time, use its system model to examine the system status at some time in the future. Although simulation-based real-time control systems are in their infancy, they show great promise for the future. Over the next years, simulation-based real-time control systems should move from 'cutting-edge' to a proven and widely deployed technology. Ideally, coupled experimental and simulation investigations should be run in parallel and in real time in order to provide the synergy between these two approaches and complimentary interpretation of the observed phenomena. It intimately connects theory to experiment for the same system under investigation. The development of the corresponding computer-guided methodologies and combined strategies that aimed at increasing efficiency of experimentation is one of the major priorities of the computationally-based sub-project.

**Possible Applications:**

- Surface specific methods: atomic force microscopy (AFM); scanning probe microscope (SPM); scanning tunnelling microscope (STM); scanning near field optical microscope (SNOM or NSOM); optical microscopy; X-ray photon electron microscopy (XPS); Auger spectroscopy.
- Transmission electron microscopy (TEM), including analytical (ATEM), diffraction, high-resolution (HRTEM) and spectroscopic (electron energy loss spectroscopy) techniques.
- Single-crystal and high-resolution powder X-ray diffraction (XRD), neutron diffraction, diffuse diffraction. (Determinations of detailed crystal structures, lattice parameter variations, role of dynamical effects, defects, etc.).
- Spectroscopic techniques, including infrared (IR), Raman, nuclear magnetic resonance (NMR), 2D-NMR, X-ray absorption (XAS), Brillouin scattering. (Characterisation of local structural variations, acoustic phonons, etc.).
- Time-dependent physical properties: ultrasonics, dynamic mechanical analysis, specific heat, electrical conductivity dielectric permittivity, bi-refringence. (Characterisation of phase transitions, time-dependent order, etc.).

## Development of large-scale scientific applications software and new user-friendly interfaces for computational tools

A major change in design and manufacturing during the past 50 years has been the growth of (computer) simulation as a design tool. It has become possible to simulate with increasing accuracy more areas of product performance. Companies have realised that this is an increasingly effective tool for providing better products at a lower cost. Nowadays, even quite mundane chemical products may be the subject of sophisticated analysis. There are enormous potential opportunities for numerous important industrial problems involving the materials sciences, biotechnology, and chemical technology. This opportunity is to design, characterise, and optimise materials before beginning the expensive experimental processes of synthesis, characterisation, processing, assembly, and testing. With reliable *de novo* simulations on real materials, industry could save enormously by cutting years off development cycles, while achieving designs that are more efficient. Moreover, such *de novo* design would allow efficient consideration of completely new materials and designs, which is particularly important for the challenges of environmentally benign industrial chemistry.

It is now commonplace to say that materials science software plays a vital role in modelling and simulation at the atomic and molecular scale. Advances in computational hardware technology have fostered continuous improvements in application methods and allow for more 'brute force' calculations using state-of-the-art supercomputers and grid computing. These improvements make it possible to study larger and more sophisticated systems and require less time to achieve simulation results. In addition, the development of low-cost computers has considerably increased the ease with which some of these simulation tools can be applied. Optimisation and simulation are two areas whose use has increased enormously since the development of the PC. Clearly, advanced software is a critical component in this field. At the same time, the complexity of the computational methods that one has to master in many types of simulations, has grown to such a level that it is quite difficult for individuals or even small groups to start such a software project from the very beginning. Computational scientists spend considerable effort developing applications for simulating complex systems. In addition to the simulation methods, various software engineering and data interchange aspects are important. As a result, existing software is often employed. Understandably, the existing simulation non-commercial packages themselves are commonly very complex and not intuitive to use. In many cases, one requires an expert knowledge of the application to use it effectively, which limits the usage of the application and thereby reduces the research impact.

Ideally, the simulation tools should be integrated smoothly with, and executed from, a user-friendly interface that enables non-expert users to access complex simulation applications. They should be coupled closely with dynamic graphical displays of structures, simulation processes, analytical data, and results, and should assist in the selection of the optimal simulation strategy, supported by a high-speed network infrastructure. In the molecular-scale simulation, a graphical user interface should incorporate tactile and icon-based capabilities for building, editing, analysing, and visualising of graphical models of molecules – from materials and chemicals to DNA and macromolecular proteins – as well as services to convert and visualise the results of simulations for the understanding of scientific models and content. Another requirement is that the simulation infrastructure be integrated with laboratory information and online measurements that fosters the interaction between simulation community and industry in the use of advanced computing technologies and laboratory equipment. The upcoming use of the Internet as mass medium also advances the development of user-friendly interfaces - new features like workspaces and multimedia applications - and supports the establishment of a global information space.

The main components of our 'developing philosophy' are outlined below:

- The development of new approaches and easy-to-use software systems for materials simulation, both on high-performance computers and on PCs.
- The development of hierarchical modelling approaches combining atomic-scale, molecular and mesoscopic modelling, as well as conventional engineering computing (Finite Element Analysis, Finite Difference Methods and Boundary Element Methods).
- For distributed computing to be viable, software must be designed and implemented as components whose services can be accessed from any other component that needs it.
- The application of the simulation software to problems of technological relevance and the transfer of the acquired knowledge into industrial research.
- The workings of complex computer programs should be as transparent as possible to help both user understanding and future development.
- A high-level of 'user-friendliness', including the presence of user-friendly interface, educational modules, and intelligent tutoring systems is desirable.
- The interface must be easily customised, allowing for spreadsheet data input and mouse-based interaction with the model.
- Simulation products must also provide for customisation through a structured language.
- A hierarchy of conveyor section types should be created in which the object-oriented concept of inheritance is provided directly to the simulation user.
- Interface to other software tools like MS Excel and CAD systems is necessary.
- The mathematical complexity of the solution needs to be masked by an interface applicable to both the power user and the average user.
- As these interfaces become more sophisticated, building and presenting models should become more intuitive.
- Output analysis tools for simulation need to include more guidance for users to prevent erroneous inferences. (The software needs to protect the non-expert user from making mistakes when interpreting the results. Additionally, the expert user needs better tools for constructing customised reports and capturing simulation information for later analysis).
- Template models can help reduce the model development time and can provide valuable insight into the appropriate inputs to be considered when analysing a given process.
- The development of a visual simulation environment (the interactive visualisation of 3D data and the visualisation of four-dimensional space-time processes).
- The design and implementation of a parallel volume and surface-oriented rendering in molecular and mesoscopic simulations.
- The implementation of scientific multimedia functionalities and distributed virtual reality into materials simulation.
- The use of high-speed network infrastructures.
- Cooperation with scientists and developers in the fields relevant to scientific visualisation.
- Bilateral cooperation between groups of the participating research institutes and industrial enterprises.

# 4 Development of Analytical Techniques

## Universal analytical methods for single molecule/entity characterisation

In order to analyse any new molecule, substance or material, there is a need to separate it from the production process mixture, or in the case of biologically generated materials, to remove it from the biological host, and to eliminate any impurities. This is a long-winded and costly exercise. One of the most important priorities therefore in the development of new analytical techniques is the successful separation of complex mixtures, e.g. on chip separation and micro Total Analysis Systems (TAS), or the *in-situ* analysis of new molecules, substances and materials, for example, the detection of drug delivery at the cellular level.

Once the molecule, substance or material has been isolated or located, it needs to be characterised in various ways. Crucial here is the determination of the chemical composition of the entity, and its 3D structure, particularly for the assembly of the materials. These requirements need to be achieved at the highest sensitivity and in the shortest timeframes possible. Examples of possible research areas in the detection of very small quantities of substances at high levels of sensitivity include: metal ion sensitive arrays, anionic fluorescence sensors, highly sensitive sensor systems, surface plasmon resonance, high-frequency mass-sensitive devices, particle and surface-enhanced Raman spectrometry, the creation and control of IR quantum dots as probes, nano-LEDs for fluorescence spectroscopy and cellular imaging and organic lasers as biomarkers. Analysis methods that have previously been restricted to one dimension need to be extended to further dimensions, for example spatially resolved functional ESR of multiple crystals. Additional frontiers that need to be explored are the analysis of non-crystalline chemical structures, and related to this, the analysis of molecules at interfaces (interface/surface analysis):

- Total surface area and thickness of interfacial area measurements.
  - Organic/inorganic interfaces (polymer/polymer, multilayer films, multiphase blends).
  - Organic/inorganic interfaces: hybrid materials.
  - Organic-inorganic/biological interfaces.
- Liquid / liquid interface: dispersion.

Of particular importance are tools for the characterisation of biopolymers and macromolecular molecules. Work on the various types of stochastic sensors, new forms of membranes for separation, novel electro spray ionisation mass spectrometry (ESI-MS) methodologies, hybridisation of existing methodologies (e.g. matrix-assisted laser desorption ionisation time of flight mass spectroscopy), time-resolved non-linear optical spectroscopy and the use of luminescence/fluorescence probes could lead to better isolation and characterisation of macromolecular entities.

Many of the existing analysis tools listed can be improved significantly:

- **Tomography in 3D (TEM, X-ray).**
  Extend the 2D measurements to the third dimension (3D). This would lead to an improved ability to quantify the spatial relationship of particles confined in a matrix, e.g. phase analysis, nanoparticles in cells.
- **Solid state 3D NMR at the nm scale.**
- **Extend solid state NMR composition analysis at the 10-100 µm to the nm scale**.
  Through the use of more sensitive probes and smart software (operator-friendly) for the interpretation of the data.
- **Microscopy and spectroscopy:**
  - SPM, SNOM (scanning near optical microscopy).
  - Scanning probe methods, scanning force microscopy.
  - Atomic force microscopy (AFM).
  - Scanning electron microscopy (SEM) methods.
  - Laser-induced fluorescence (LIF), laser-induced incandescence (LII).
  - Electrospray mass spectrometry (ESMS), nanospray mass spectrometry (NMS).
  - Coherent anti-stokes Raman scattering (CARS).
  - Emission spectroscopy.
  - Adsorption.
  - Three-dimensional medium-energy ion scattering spectroscopy (3D-MEIS).
  - Nanodiffraction.
  - High-resolution imaging (HREM).
  - Pulsed Field Gradient (PFG) Nuclear Magnetic Resonance (NMR) spectroscopy.
  - Monitoring the diffusion within the pores of nanomaterials.

**Pulsed Field Gradient Nuclear Magnetic Resonance spectroscopy.**

The PFG NMR method relies on recent progress in diffusion measurement by the nuclear magnetic resonance technique, which enables the assessment of the transport properties of porous catalysts during the fabrication process. Catalyst production involves synthesis of microporous materials and the modification of the catalysts by varying extraction, substitution, steaming and formulation conditions, which result in the formation of specific pore networks that accompany demetallisation of the porous lattice. Structure characterisation focuses on the chemical nature of the catalysts and the hierarchy of the intrinsic pore system. Catalyst testing is a prerequisite to provide key numbers for catalyst yield, selectivity, environmental compatibility and durability in, for example, fluid catalytic cracking (FCC), which is one of the most celebrated fields of industrial application of heterogeneous catalysis. Correlating the transport properties with the corresponding features of catalyst production, structure and performance, molecular modelling ensures the elucidation of those features of catalyst production that – because of their favourable influence on transport properties – guarantee high-performance porous catalysts. The development of novel fabrication routes requires interdisciplinary contact between end-users with expertise in the application of catalysts, catalyst manufacturers with expertise in catalysis synthesis, modification and formulation, and experts in fundamental research in the fields of structure characterisation, diffusion measurement and molecular modelling.

## High-throughput analysis

The rapid and reliable online detection as provided by chemical sensor techniques for analytes, ranging from chemical compounds up to entire microorganisms, has become a 'hot topic' within the scientific community during the last two decades. However, the design of outstanding selective sensor materials (e.g. artificial antibodies) that combine selectivity analogous to biological systems with the ruggedness, stability and processability of man-made materials still remains a challenge. In addition, Europe will strongly have to support the development of novel, miniaturised transducers to achieve increased sensitivity and stability of the analytical systems. At the moment, sensor technology mainly points at two tasks: establishing true distributed analysis mainly for environmental purposes (e.g. by designing radio-controlled analytical stations that are centrally surveyed), and (industrial) process control to ensure high economic and ecological sustainability of production processes. Thus research has to emphasise:

- Novel, nanostructured functional materials for sensing purposes.
- Design of highly sensitive transducers.

Techniques which will support the analysis of combinatorial chemistry, will play a vital role in the future. The demand for new analysis methods in the field has become so large that books reviewing the field are beginning to emerge. But not only on the large-scale are these demands being met, the field of high-throughput protein glycomics and protein separation on chip promises a bright future. There still remain areas which need pioneering work:

- Parallel analysis.
- Separation of highly complex systems.
- Monitoring of nanoobjects, or composites thereof, for industrial production consistency (LASER, acoustical techniques).
- Automated sample preparation (for TEM, AFM).
- Combinatorial chemistry applications.
- Introduce 'chemical' information into scanning probe techniques by extending the capabilities of current AFM/STM systems.

## Nanomaterials

In the field of nanomaterials, not only is there a need to be able to analyse individual components, but also the properties of the whole system at the macroscopic level, which is built upon the inherent properties of the nanoscale components. Therefore a correlation between the spatial organisation and fundamental property information at nanoscale (e.g. mechanical, chemical, thermal, etc.) needs to be discerned by the analytical method. For research and industrial processes, there exist a number of analytical techniques dedicated to the analysis of nanomaterials. These can be categorised into four disciplines (with the related analytical technique listed below):

- **Determination of atomic structure and chemical composition:**
    - Spectroscopic methods.
        - Vibrational spectroscopy: Fourier Transform Infra Red (FT-IR) and Raman Scattering.
        - Nuclear Magnetic Resonance: liquid and solid-state.
        - X-ray and UV-vis spectroscopy.
    - X-ray and neutron diffraction.
- **Determination of size and shape:**
    - Electron microscopies.
    - Scanning Electron Microscopy (SEM).
    - Transmission Electron Microscopy (TEM).
        - TEM is not capable of characterising H and C structure at nm scale.
    - Brunauer Emmet Teller (BET) and Helium Pycnometry.
    - Epiphaniometer.
    - Laser granulometries and Zeta potential.
    - Elliptically polarised light scattering.
- **Detection of nanomaterials in aerosols:**
    - Condensation Particle Counter (CPC).
    - Dekati Low Pressure Impactor (DLPI).
    - Electrical Low Pressure Impactor (ELPI).
    - Scanning Mobility Particle Sizer (SMPS).
    - Scanning Transmission Electron Microscopy (STEM).
    - High-Resolution Transmission Electron Microscopy (HRTEM).
    - Scanning Probe Microscopy (SNOM and AFM).

- **Detection of nanomaterials in biological tissue :**
  - Cryogenic Transmission Electron Microscopy (C-TEM).
  - Scanning Transmission Ion Microscopy (STIM).

There is, however, a lack of analytical standards for nanomaterials; neither have the environmental, health and safety (E&HS) issues been resolved. This can be addressed by developing:

- **Standard/reference nanomaterials.**
  For characterising size and shape, especially plate-like and rod-like (spherical standards have already been developed).
- **Test protocols for structure-property relationship, size and shape.**
  To be able to compare raw materials with the final composites or products.
- **Detection of nanoparticles in biological matrices.**
  E.g. assess impact of nanotubes, buckyballs on cancer growth.
- **Mode of entry/exit of nanoparticles into the biological systems.**
  Needed to determine worker exposure limits and biological decomposition.
- **Method for aerosol generation of un-agglomerated nanoparticles.**
  To date one cannot study the EH&S impacts of single nanoobjects because they agglomerate.
- **Methods to study nanoparticle dissolution in biological fluid.**
- **Toxicology and test methodologies.**
- **Persistence.**
- **Nanoparticle detection methods and tools.**
- **Modelling that correlates structure, composition, surface chemical state and properties to biotoxicity.**

### Analytical norms and standards

There is a need to have a coherent and comprehensive set of norms and standards that can be applied, at least Europe wide. This could be achieved by the formation of an independent European authority, which supervises the implementation of norms, develops new standards on consultation and assists in their implementation. This authority could provide Europe with an edge over the other competing markets (USA, Asia, etc.) by having these norms and standards in place in a quick and efficient manner, and by setting the tone for the kinds of norms and standards needed, particularly in the field of nanomaterials. It is important that, when norms or standards are being developed, they are derived in a case-by-case manner, to address adequately the particular conditions and circumstances relevant to each case. Industry can contribute significantly to the development of norms, particularly when these norms are voluntary, by giving comments as to whether norms should be rigid or flexible, more descriptive than performance-based. Obviously, those who participate in developing norms, have the benefit of securing their interests and technological advantages. Norms play an important role in the competitiveness of businesses; they help in standardising the requirements for production processes, provide a means to compare quality control criteria; they serve as a verification of quality, provide legal security by reducing liability and can unburden the legislator where laws and ordinances have be waived due to the existence of good norms and standards[6]. It is with this background that the following propositions should be considered:

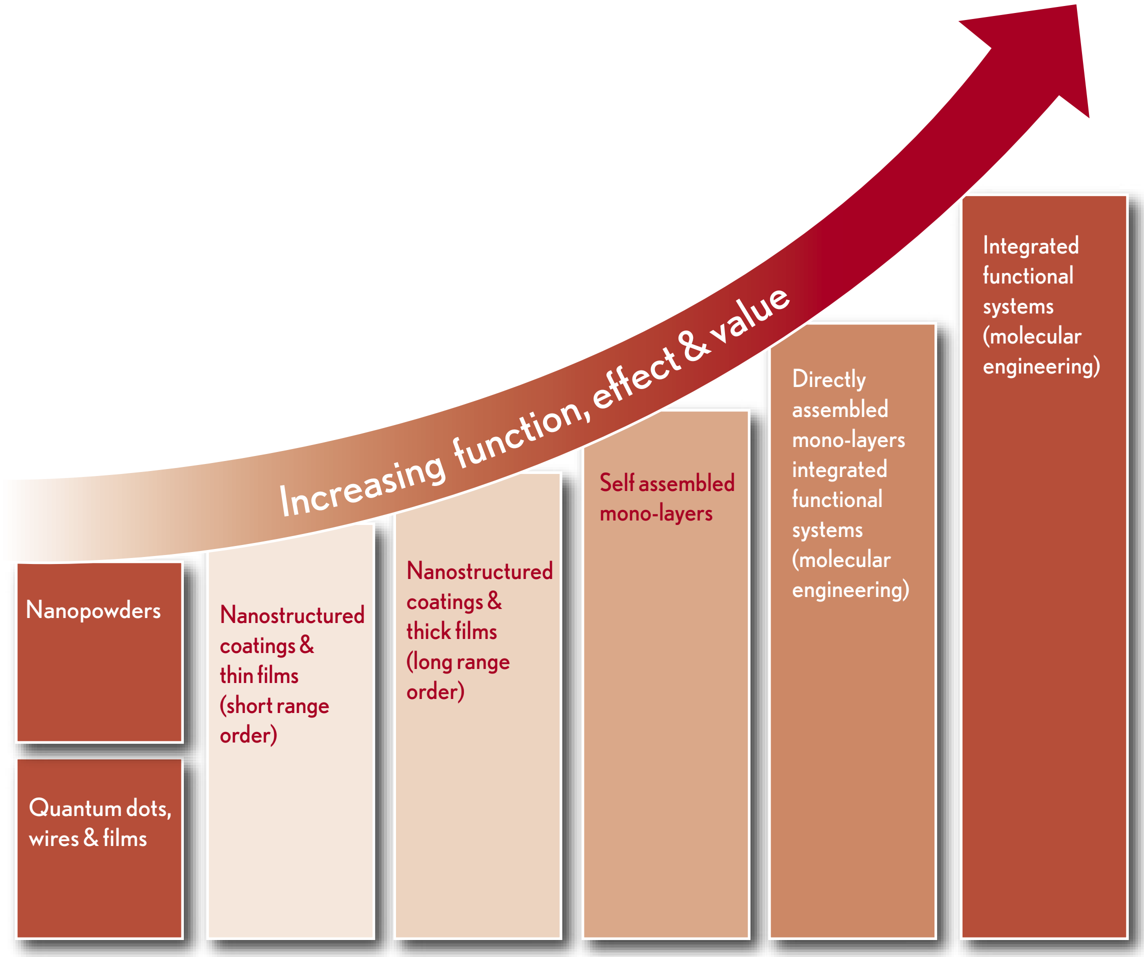
- **The formation of a European Norms and Standards Agency.**
- **The development mechanisms for the adequate definition of new norms and standards for nanomaterials.**
- **The development of instruments to encourage the involvement of industry and relevant stakeholders in the development process of norms and standards.**

## 5 From Laboratory Synthesis to Large-Scale Manufacturing

In order to realise the potential of nanomaterials in everyday products, a number of technology scale-up processes need to be realised. This is illustrated in the 'Innovation chain' illustrated below in Figure C.1.

In the realm of current conventional technologies, the adaptation of synthesis processes to include novel gas phase processes, e.g. plasma- or microwave-assisted processes; or novel wet processes, e.g. sol-gel processes, for the manufacturing of nanomaterials need to be addressed immediately. Further new dispersion and stabilisation, *in-situ* functionalisation and formulations, and integration in patterned and final system construction processes need to be pursued. But beyond this 'step-out', technologies such as self-assembly, self-organisation (with long-range order) and the *in-situ* generation of nanostructured materials must be contemplated.

*Figure C.1: Innovation chain for nanomaterials*

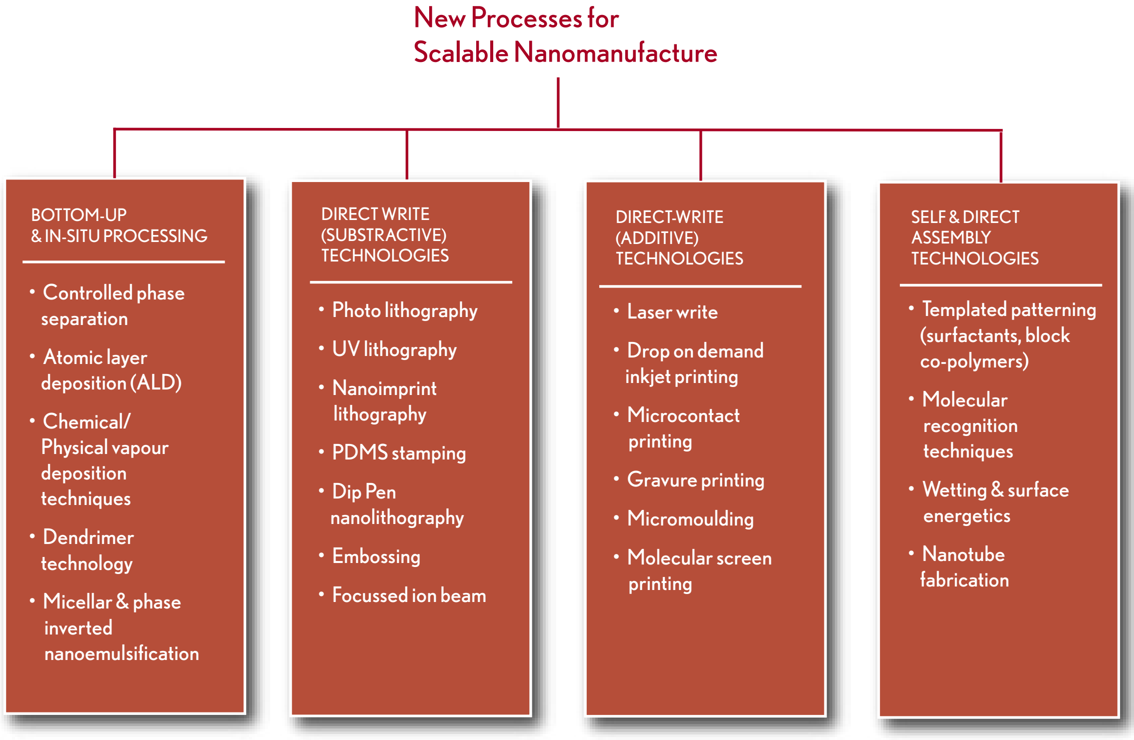


To meet market demands, both conventional and step-out technologies will have to have a scalable design for manufacturing, as detailed in Figure C.2. These new modular technologies can be categorised into:

- Bottom-up and *in-situ* technologies.
- Subtractive direct write technologies.
- Additive direct write technologies.
- Self- and direct-assembly technologies.

Crucial aspects beyond the scalable production processes are the synthesis and processing of ultra-pure materials. Here it is important to glean an understanding of and enable the manipulation of reactions, nucleation processes, and the formation of materials through the dispersion, modification, and functionalisation of nanomaterials at the large-scale. Furthermore, the reproducibility, accuracy, and reliability of these processes should be at the level of, or better than today's, electronic manufacturing standards.

*Figure C.2: Modular toolkit for scalable manufacturing*



The production of quantum and hybrid materials poses a challenging question. Here, the development of an 'innovation toolkit' based on quantum-scale phenomena, for example transport, optical, electronic and biocompatible properties, is essential. Ensuring that these unique properties of quantum materials are maintained from the synthesis through to the final integrated system is a demanding activity. Furthermore, molecular engineering of complex hybrid materials and their fabrication needs to be developed.

One current production technology that through adaptation for nanomaterials, would lead to new flexible functional materials is the 'reel-to-reel' manufacturing process. This would enable the production of flexible and large area electronics and conformable solar cells. Furthermore, the transfer of patterning techniques from small-scale lab production processes to 'reel-to-reel' manufacturing technologies would have a significant impact on future products and markets.

The development of embedded devices and systems for use in sensing, actuating and responsive materials (based on basic principles) relies on the inclusion of built-in tiny energy supplies. This poses a considerable challenge for the large-scale production processes.

Aside from the development of physical production processes, there is a need for the development of software tools for optimising cost versus scale-up, but especially for performance. When connected to inline and online nanometrology tools (see *Analytics*), these software tools should be able to maintain optimum production levels.

By 2025, scale-up processes and technologies should have adapted the following principle:

*smart synthesis + patterning = function by design*

## 6 Bio-based Performance and Nanocomposite Materials

Using the knowledge obtained from fundamental research, it should be possible to develop bio-based materials for the following applications:

- **Controlled release of drugs and nutrients.** Bio-based materials show a higher biocompatibility and are therefore ideal carriers to be administered to human beings. Research should be focused on tuning the properties of the materials, like biostability and biodegradability. New and better systems for the encapsulation of drugs and nutrients have to be developed. Novel concepts are needed to respond to physicochemical changes that can trigger the release of the encapsulated compound. For instance, the pH near a cancer cell is slightly lower than near healthy cells; a carrier could be made that responds to these minute pH changes and then releases the drug. The controlled release of nutrients has been deliberately included here. Curing diseases is an end-of-the-pipe solution, and since the average age in Europe is increasing, one cannot afford to only focus on ill people: one has to prevent illness by the administration of health-improving, disease-preventing compounds. Also these compounds have to be carried and released at the right target spot. Another application of materials for controlled release will be personal care products.
- **Biomaterials as healing dressings and/or scaffolds in tissue engineering.** Some biomaterials such as bacterial cellulose or chitosan are known as healing dressings. However, the wound healing process can be increased or accelerated by simultaneous application of bioactive compounds (nucleotides, oligopeptides and some lysophospholipids), which can act as ligands for cell surface-bound receptors involved in signal transduction. The binding of such compounds (or ligands) to these receptors can stimulate the proliferation of keratinocytes, fibroblasts, endothelial cells and other cell types which are involved in the wound healing process. Research should be focused on the use of biomaterials as carriers for ligands stimulating cell membrane receptors and on controlled release of these compounds. One can also consider chemical modification of existing biomaterials to obtain new generation of healing dressings. Such modified biomaterials can be used not only as the healing dressings but also as scaffolds for *in-vitro* cell culture or tissue engineering. Tissue growth is strongly stimulated when a suitable scaffold is present; when the mechanism is known by which the cells recognise their solid substrate, one can devise biopolymers (which should be self-decaying in a few months) that can act as a template for the new tissue.
- **Biomaterials for artificial hybrid organs.** It would be advantageous to develop biomaterials with specific properties that protect transplanted allogenic or xenogenic cells against the immune system of the recipient, avoiding the use of immuno-suppressants.
- **Smart packaging materials.** To date, the purpose of packaging was mainly to protect the contents against dirt, contamination and/or oxidation. It would be useful to devise packaging materials that act as sensors, for example, materials that respond to the decay of meat. This would be a more reliable indicator of food quality than a general indication of shelf life on the packaging.

- **Eco-friendly antifouling coatings.**
  The attachment of various forms of sea life to boats is a serious problem that is countered by the use of toxic chemicals. This could be circumvented if one could coat the vessels with a material that prevents this. This is an application where the repellent properties of biological molecules are of importance; if one understands the mechanism of molecular recognition, one can also design a system that will repel cellular components. Antifouling is also an important topic in membranes, which are used for industrial separation processes.
- **Smart materials (e.g. membranes, adsorbants) for separations of (bio)molecules.**
  They can be used for desalination, the removal of pollutants from water, or the removal of malodours from foodstuffs. Alternatively, they can be designed in such a way that the product of a (bio)chemical reaction is removed from the reactor, in order to shift unfavourable reaction equilibrium to the desired side, or to separate a desired (bio)molecule from a diluted solution. Nature is again a source of inspiration here: the cell membrane has many mechanisms for the controlled complexation and transportation of (bio)molecules. The molecular recognition phenomena involved should be utilised for the development of the smart bio-based separation processes.
- **Smart surfaces and matrices for the immobilisation of enzymes and receptors**.
  Enzymes are the 'workhorses' of industrial biotechnology, and for various reasons it is important to immobilise them onto a solid support. At present, enzyme immobilisation is a more or less random process; it would be advantageous to have surfaces and matrices that interact with the enzyme in such a way that the non-catalytic part of the enzyme is bound to the surface, leaving the catalytic site open to the solution, in order to ensure optimum activity. Also receptors should be immobilised in such a way that their recognition capacities are unaffected. An example could be the use of structural polypeptides as spacers for immobilisation of different enzymes at distinct positions to allow sequential reactions, or catalytic polymers. The developed materials and techniques should be applicable to nanosized channels and reactors. One could think of peptide nanotubes or natural silk textiles (fibroin) as solid supports for enzymes immobilisation.
- **Self-cleaning surfaces.**
  An application could be coatings for windows so that they are cleaned by sunlight and rain, or stain-resistant coatings for clothes. Taking this one step further, one could think of self-repairing coatings, like in self-repairing paint. This relates again to living systems, which are able to repair themselves using self-assembly. Can this be translated into 'non-living' systems?
- **Self-organising polymers.**
  These could act as templates or moulds for electronic devices, or as memories. As fabrication using conventional top-down approach reaches its theoretical limit, bio-based bottom-up self-assembly could allow the fabrication of electronic devices in the scale of 10-20 nm.
- **Hard- and software for analysis.**
  Molecular recognition as an interface between the PC and biological activity. Communication using electrical signals is very common in biology (e.g. ionic current or electron transfer). Many recognition and identification events could be translated into electrical and electrochemical signals that will allow the computer-biomolecular interface to evolve.
- **New biomaterials with properties that were considered 'impossible' in the past.**
  Some of the self-assembled biomaterials have remarkable physical properties (e.g. spider silk is stronger, yet much more flexible than steel). The understanding of the molecular basis for self-assembly can allow the design and manufacture of materials with unique properties. Another example could be a combination of antimicrobial activity and selective binding to specific tissue cells or injectable materials, which can be used to repair or strengthen damaged or weakened tissue, for example, treatment of stress incontinence and use in plastic/cosmetic surgery. Natural composite materials with exceptional toughness, such as nacre ('mother-of-pearl') could also serve as a source of inspiration for the design of novel organic/inorganic nanocomposites. These materials should be (largely) bio-based or at least bio-inspired. This means that they are composed of bio-based building blocks, designed using principles derived from biopolymers, or made by enzymatic modification of biopolymers.

## 7 Synopsis

Having presented the topics that are considered important to provide the impetus for the innovation of new materials and products, the following illustrations give an impression of the scope of influence that material technologies have, not only within SusChem, but also in relation to the other technology platforms (figure C.3).

Within SusChem there are naturally a large number of themes where an overlap between the *Material Technology* section and the *Reaction and Process Design* section occurs as illustrated on page 77 of the SRA (figure 7.1). For instance in:

- Functional coatings.
- Synthetic concepts.
- Process intensification.
- Materials for catalytic transformations.
- Purification and formulation engineering.
- *In-silico* techniques.
- Plant control and supply chain optimisation (integrated systems).

The relationship to industrial biotechnology rests rather on the materials produced (see figure B.1 on page 32 of this document):

- Bio-based plastics.
- Advanced polymers.
- Bio-inspired materials.
- Bioelectronics.
- Miniaturised structures.
- Barrier properties.
- Chemical/physical sensing.
- Multi-thin layer structuring.

*Figure C.3: Material technologies connections to other technology platforms*

| Technology Platforms | Fundamental understanding of structure property relationships | Computational material science | Development of analytical techniques | From laboratory synthesis to large-scale manufacturing |
|---|---|---|---|---|
| ENIAC - Nanoelectronics | 🟥 | 🟥 | 🟥 | 🟥 |
| EuMat – Advanced materials |  | 🟥 | 🟥 | 🟥 |
| ESTP - Space technology |  | 🟥 | 🟥 | 🟥 |
| Nanomedicine |  |  | 🟥 | 🟥 |
| ACARE - Aeronautics |  | 🟥 | 🟥 | 🟥 |
| Photovoltaic |  | 🟥 | 🟥 | 🟥 |
| ARTEMIS - Embedded systems |  | 🟥 | 🟥 | 🟥 |
| eMobility - Communication | 🟧 | 🟥 | 🟥 | 🟥 |
| Innovative medicine | 🟧 |  | 🟥 | 🟥 |
| FTC - Textiles and clothing | 🟧 | 🟥 | 🟥 | 🟥 |
| Hydrogen fuel cells | 🟥 | ⬜ | 🟥 | 🟥 |
| Manufuture - Manufacturing | ⬜ | ⬜ | 🟧 | 🟥 |
| ECTP - Construction | ⬜ | ⬜ | 🟧 | 🟥 |
| TP Safety - Industrial safety | ⬜ | 🟧 | 🟥 | 🟥 |
| Food for life | ⬜ |  | ⬜ | 🟥 |
| WSSTP - Water supply |  | 🟧 | 🟧 | 🟧 |
| GAH – Animal health |  | 🟧 | 🟧 | 🟧 |
| Coal and steel | ⬜ | ⬜ | 🟧 | 🟧 |
| WATERBORNE | ⬜ | ⬜ | 🟧 | ⬜ |
| ERRAC – Rail | ⬜ | ⬜ | 🟧 | ⬜ |
| ERTRAC – Road transport | ⬜ | ⬜ | 🟧 | ⬜ |
| FTP – Forest resources | ⬜ | ⬜ | 🟧 | ⬜ |
| NEM – Electronic media |  | ⬜ | ⬜ | 🟧 |
| HTR-TN – Gas cooled reactors | ⬜ | ⬜ | ⬜ | ⬜ |
| Plants for the future | ⬜ | ⬜ | ⬜ | ⬜ |

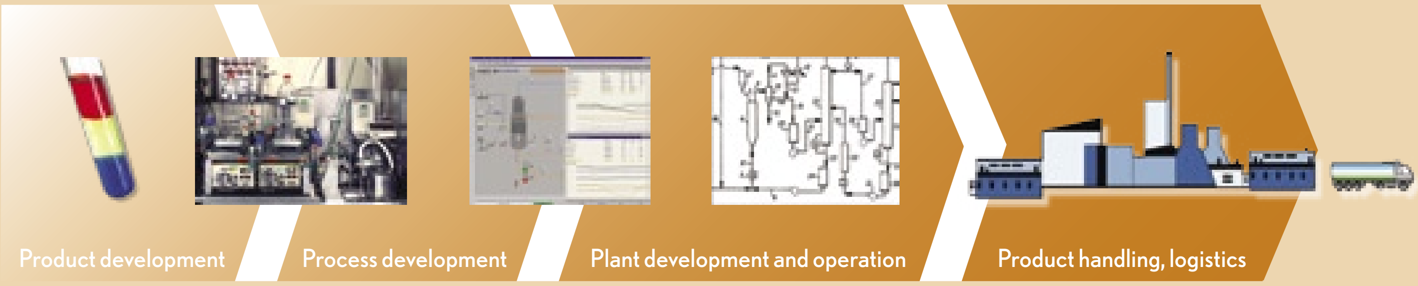
| Relevance |  |
|---|---|
|  | ⬜ Low |
|  | 🟧 Medium |
|  | 🟥 High |

# Reaction & Process Design

## 1 Introduction

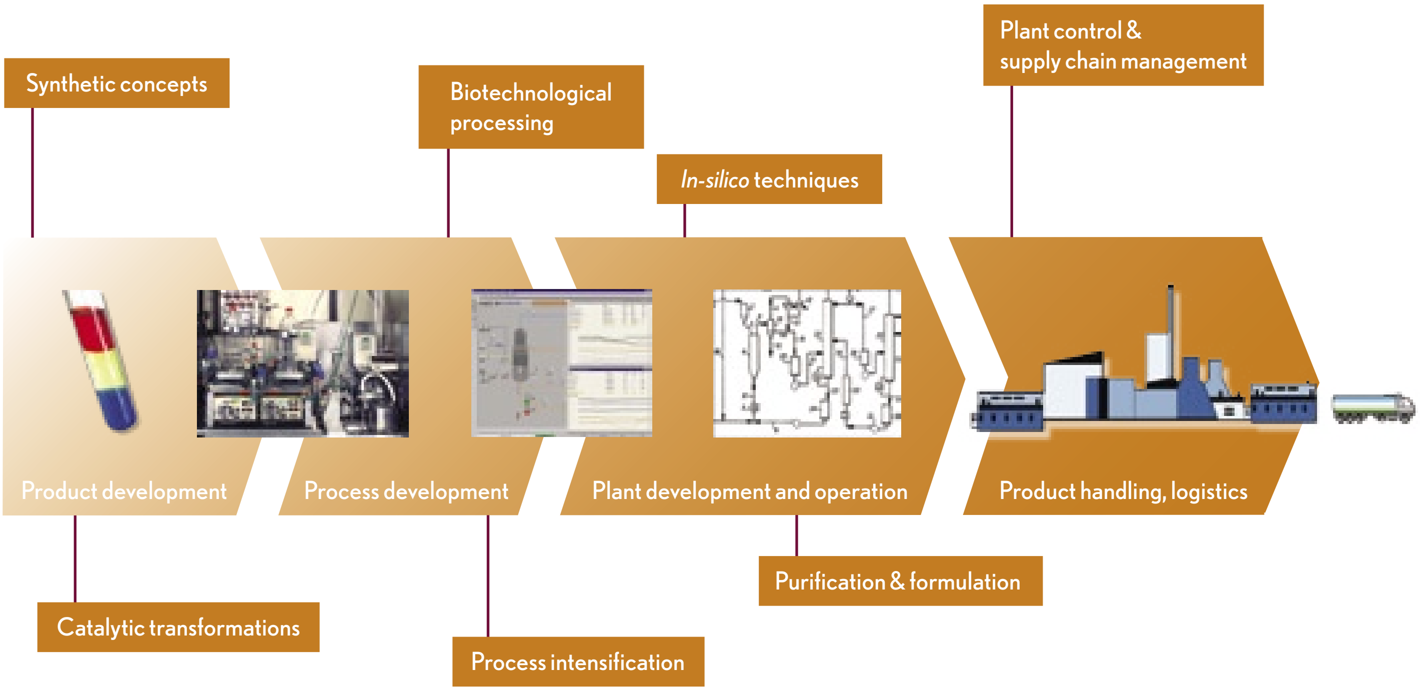
The way one manages the valuable natural resources, designs industrial products and processes, safeguards human health, or grows food, is undoubtedly influenced by how one uses material resources. In order to achieve sustainable development, a lot of progress is needed in the application of science for the identification, design and the development of appropriate products and processes that will produce them. On this note, the field of reaction and process design represents the fundamental enabling technology contributing to the entire lifecycle of processes, ranging from product development through process development, plant development and operation, to product handling and logistics. Integration of the complementary approaches of chemical synthesis and process design and engineering can be applied to all areas of chemistry and biotechnology, thus providing key contributions to all the relevant steps, from reaction to viability of process plants.

*Figure D.1: The process lifecycle*



Reaction and process design aims at processes designed from the start to incorporate: highly efficient, inherently safe and environmentally benign technologies; tailor-made products with designed properties making efficient use of (e.g. renewable) resources; smaller size facilities based on process intensification technologies with maximised reuse of materials; equipment that is geared for multiple usage and purpose, thus increasing flexibility and decreasing costs; and chemical plants that are equipped with appropriate control systems for the reactions they process. Hence, reaction & process design should be considered as the main driver for sustainable development of the European chemical industry, and for fostering innovations, which directly address the needs of the society in terms of, for example, energy, transportation, environmental protection, healthcare and quality of life.

*Figure D.2: Reaction and process design research priorities: contributions to the entire process lifecycle*



The *Reaction and Process Design* section of SusChem identified the following seven **priority fields of research**, which have particular impact on the objectives and societal needs mentioned above:

- **Novel synthetic concepts** aim at cost-effective new synthetic pathways with a reduced number of steps, higher energy efficiency, lower raw materials consumption and avoidance of by-products and waste. Specific approaches utilising alternative, especially renewable, feedstocks to create a broad slate of different chemicals will start to supplement chemical production, starting from classical oil refineries, thereby reducing dependency on oil as the dominant raw material.
- **Catalytic transformations** specifically enable chemical processes to be realised in a cost-, energy-, and eco-efficient way. Catalysis provides key contributions to sustainable mobility, clean fuels production, the rational use of resources including alternative raw materials, sustainable energy (fuel cells, use of solar energy), and environmental protection (air and waste water purification, solid waste reuse, reduction of greenhouse gas emissions, soil and water remediation).
- **Biotechnological processing** aims at e.g. the combination of genetic engineering methods and analytical high-throughput processes to considerably speed up biocatalyst and process development, thereby enabling economically competitive bioprocesses with the potential to complement or even replace chemical processes, and also to pave the way for new products.
- **Process intensification** aims at the reduction of process steps as well as use of novel and more eco-efficient synthesis routes enabling greater production with smaller/cheaper equipment, less energy consumption, smaller quantities (or even absence) of solvents, substantially lower risk, reduced environmental impact and higher selectivity for similar or even higher conversions of reactants.
- ***In-silico* techniques**, driven by accelerating developments in high-performance computing, chemical sensing technology and distributed process control, result in design of new catalytic and/or multifunctional materials, enhance operational efficiency of industrial processes and enable the development of flexible processes suited for the production of a wide range of products in a single unit.
- **Purification & formulation** processes support zero-emission plants producing purer products conditioned to suit market needs. They strongly alleviate the impact of the chemical industry and products on the environment and human health. Innovative technologies will enable cheap purification of substantial product streams, thereby reducing energy and material consumption by 25% and achieve zero-waste production for at least 20% of existing technologies.
- **Plant control & supply chain management** aim at a production and business paradigm shift towards knowledge-based, model-centric manufacturing, subsequently strongly increasing efficiency and flexibility of the European chemical industry. Advanced plant control, process performance monitoring and supply chain management result in flexible, inherently safe production plants with optimal market demand responsiveness.

All of these strongly cross-cutting research priorities have tremendous impact on many sectors beyond the chemical industry and address different aspects of life.

The market impact of reaction and process design and the financial need for its development is difficult to assess. If one takes the € 580 billion estimated chemical production per year for 2015, and conservatively assumes 30% of this production value is influenced by R&PD, and again assumes cost savings compared to existing technology at 20%, the additional value generated would be € 35 billion per year. If one targets at 3% R&D spending of sales, this should require research activities worth about € 1,050 million per year, i.e. € 7.35 billion over the seven years of FP 7. The commission should consider contributing 15% of this spending, amounting to roughly € 1.1 billion, for the research activities within reaction and process design over seven years.

# 2 Synthetic Concepts

## Challenges

Devising novel synthetic concepts is a continuous research task in chemistry. The major challenge in this field is the need to step out of the conventional framework of thinking, both with respect to reagents and with respect to process conditions, in order to achieve breakthrough improvements. Novel concepts need to be generic and broadly applicable to allow practical implementation. Most synthetic concepts will rely on catalytic transformations, and therefore cross-fertilisation between these two fields is highly desirable.

## Scope

Novel synthetic concepts cover the whole range of chemistry, including novel transformations, application and production of alternative feedstocks, new reaction media and reaction conditions, and/or innovative cheaper, shorter or more benign pathways to known products. Synthetic concepts however, can never be considered isolated, but have to be developed in parallel with equally advanced reaction engineering concepts. Novel synthetic concepts could therefore benefit especially from advances in catalysis and process intensification.

### Vision

New cheaper synthetic solutions with a reduced number of steps, based on innovative energy sources (like microwaves, plasma), new solvents and reagents (like water and ionic liquids) and new reactor concepts, are available for industrial implementation in many fields, providing energy-efficient and waste-free routes to a wide range of target molecules and taking advantage of novel feedstocks hitherto unused in chemistry. Renewable feedstocks will form the raw materials basis for 'biorefineries', in which a broad slate of different chemicals is created and which will start to supplement the chemical production starting from classical oil refineries.

## Goals - rationale and objectives

Novel synthetic concepts should either allow the synthesis of known targets in a more efficient way, which means with reduced energy input and reduced waste output, or tap novel feedstocks hitherto unused in chemistry. Instead of specialised synthetic procedures adapted to a specific transformation, generic solutions should be provided. This should be supplemented by methods which allow a priori adaptation of process conditions, if novel substrates are to be transformed.

Novel synthetic concepts range across all sub-disciplines of chemistry and will influence not only chemistry, but also other areas. In order to reach the goals of improved efficiency, one will need completely new synthetic approaches for a given target molecule, or the same functionality could be achieved by a compound which is easier to make. Changing the feedstock basis could entail redesign of value generation chains. Innovations such as reduction of solvent use, alternative forms of energy input, or simpler oxidants could all contribute to the development of energy-efficient and waste-free processes.

The market impact of such novel synthetic concepts and the financial need to develop them is difficult to assess. If one takes the € 580 billion estimated chemical production per year for 2015, and conservatively assumes 10% of this production value replaced by novel synthetic concepts, and again assumes cost savings compared to existing technology at 20%, the additional value generated would be € 12 billion per year. If one targets at 3% R&D spending of sales, this should require research activities worth about € 360 million per year, i.e. € 2.5 billion over the seven years of FP 7. The commission should consider contributing 5% of this spending, amounting to roughly € 125 million for the topic of 'Synthetic Concepts'.

## Research priorities and roadmap

Research in the following directions is particularly important in order to meet the economic and environmental challenges that chemistry is facing in Europe in 2025:

- Substitution of organic **solvents** with water, supercritical fluids, ionic liquids, or the development of solvent-free processes. Organic solvents are the major waste load in many processes, and their replacement will both be environmentally highly beneficial and much more economical.
- Use of **novel building blocks** for synthesis, such as $CO_2$. This serves actually two purposes, i.e. reducing the released amount of a greenhouse gas and replacing toxic reagents, such as phosgene. Short-term targets are syntheses replacing phosgene; in the long run, broad application of $CO_2$ as $C_1$ building block or direct dinitrogen activation should be targeted.
- Introduction of **novel feedstocks** based on biomass. Biomass contains pre-formed fragments of target molecules, so that pathways could become available with a reduced number of steps. In addition, increasing use of biological feedstocks reduces the dependence of the chemical industry on oil. Short-term targets would be syntheses starting from glycerol, since this is a by-product of biodiesel production. In the long run, a broad range of different biomass derived feedstocks will be used for chemical production.
- **Reducing the dependence on oil** by conversion to gas and/or coal as the raw materials for chemicals. With oil prices steadily climbing, also other alternative feedstocks, such as gas and coal, could become very attractive. Europe should prepare to tap into these raw materials for chemical production*. Short-term targets are direct oxyfunctionalisation processes for methane; long-term research should focus on energy-efficient and clean technologies for making use of gas and coal in chemical production.
- Improving efficiency by **smart synthesis**, design and reduction of the number of reaction steps. Although in many cases, for instance in large-scale production, syntheses are already close to the optimum, in fine chemistry there is tremendous room for improvement in the efficiency of syntheses by redesigning the pathways to the target molecules. If this leads to a reduced number of synthetic steps, this is typically even more beneficial. Another efficient way to address the issue of reducing the number of reaction steps is the development and use of integrated multicomponent chemical processes. A sequence of synthetic steps is converted into a one-pot multicomponent process where three or more reactions take place in a perfectly controlled and ordered way. No time-consuming and waste-producing purification of single chemical intermediates are necessary, compared to the classical stepwise alternative synthesis, where each reaction step is carried out separately and each reaction product is separated and purified. Short-term targets are the improvement of fine chemistry synthetic routes, for instance by introducing catalytic steps instead of stoichiometric ones. On the longer time scale, also large-scale processes should be reconsidered and possibly redesigned.
- Development of generic methods for the introduction of **chiral centres** in an effective way. For many drugs and agrochemicals, the introduction of chiral centres is of crucial importance. Generic methods, preferably catalytic, for the creation of such centres with a broad substrate range, would have a very high impact. Hydrogenations are already well developed; short-term research should focus on increased substrate ranges. On a longer time scale, practical stereoselective oxidations or C-C coupling reactions are highly desirable.

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* This should include a strategic move towards setting up European energy supply companies to market such products as fast as possible and at competitive prices, to stimulate a fast changeover to renewable resources (cover the whole value chain from within Europe)

- Increased use of benign and **easy-to-handle oxidants**, such as hydrogen peroxide or molecular oxygen. This will almost invariably mean introduction of new catalytic steps. The use of peracids or inorganic salts for oxidation produces by-products which are often difficult to dispose of and should thus be avoided. The short-term focus should probably be placed on hydrogen peroxide; in the long run, oxygen seems to be the desirable oxidant.
- Using **innovative means for energy input**, such as plasma technology, microwaves or light, which may also allow novel reactions. Thermal activation, if often less specific than more advanced methods of energy input, should also be more broadly explored. On a short time scale, the fundamental effects of using such methods need to be studied; the long-term goal is the introduction of these methods into commercial practice where useful.
- Development of experimental and theoretical concepts to efficiently adapt synthetic methodologies to **new substrates**. Many synthetic methods are nowadays only suitable for a limited range of substrates. If one could develop theoretical concepts to allow the expansion of the substrate range, innovation in chemical synthesis would speed up tremendously. Alternatively, high-throughput experimentation provides the means for the strongly accelerated adaptation of processes to new substrates. Since high-throughput experimentation is already beginning to be adopted by the chemical industry, use of this technology is the short-term objective, while theoretical concepts will become available on a longer time scale.
- **Elimination of protection group strategies**. The necessity to protect and deprotect functional groups adds significantly to the number of steps necessary to reach a synthetic target. It reduces yields and leads to increased waste production. More specific transformations, which only affect the desired functional groups, are urgently needed. As stated above in the paragraph on elimination of organic solvents, this is a continuous effort which cannot be divided in short and long-term goals.
- Development of **short contact time processes** which have higher space-time yields will be adapted to more intense processes. This could also allow the conversion of batch processing to continuous processes in small-scale devices. Initially, suitable chemistries have to be developed, while process implementation is the long-term goal.

Novel synthetic concepts also include the conversion of production processes based on classical chemical transformations to biotechnological pathways where these are more efficient. Such approaches are covered more in detail in a different section of this chapter.

### Key enablers, linkages, constraints

The goals formulated above require cooperation across the sub-disciplines of chemistry and between industry and academia. An important step has already been made in the formulation of a research agenda which is common for all stakeholders. The manner in which each of the tasks is tackled will vary. However, it is clear that substantial progress can only be reached if the tasks are broken down into manageable work-packages that can be addressed by small, powerful teams instead of large networks. In these teams, industry and academia should be equally represented, and exchange of staff between the two sectors would be highly desirable.

Interaction between academia and industry needs to be further strengthened, so that there is good communication between industry and academia of industry's needs and of academia's innovative concepts. Difficulties in the introduction and development of new concepts will be encountered if the conditions for chemical production in Europe become more unfavourable, since high research intensity will only be maintained in world regions where there is also strong chemical production.

## 3 Catalytic Transformations

### Challenges

Next-generation catalysts should contribute towards the achievement of zero-waste emissions and selectively use the energy in chemical reactions. They will also enable the development of new biomimicking catalytic transformations, new clean energy sources and chemical storage methods, utilisation of new and/or renewable raw materials and reuse of waste, solving of global issues (greenhouse gas emissions, water and air quality) and realisation of smart catalytic devices for health protection and the improvement of the quality of life.

Solving these challenges for the future requires the development of common scientific bases which allow a change in the approach from the search of an individual solution to the design and synthesis of tailor-made catalysts, and the development of a true technological platform to be used by several industries.

### Scope

In the shorter term, research on catalytic transformation should provide new catalytic materials and reactions, by optimising the integration between expertise, knowledge and fast screening-oriented methods. In the longer term, a non-evolutionary change is necessary with a holistic integration of the different areas of catalysis and by putting knowledge-based catalyst design at the heart of development.

**Vision (catalytic transformations in 2025)**

Catalysts will be based on the concept of catalytic nanofactories (nanosized-tailored sequence of active centres as in a production line) and of catrobots (multifunctional sites with vectorial transport of reactants). Energy will be supplied locally as needed.

Biomimicking catalysts and integrated chemical/biocatalytic processes will break down the productivity limits of current enzymatic processes, while maintaining the same energy and atom efficiency, and enantioselectivity.

### Goals - rationale and objectives

The research goals for the period 2007-2015 should focus on the realisation of the conditions to turn the vision into industrial reality, strengthening fundamental research as the basis to push innovation in an area characterised from a widespread range of applications and already industrially-oriented research.

Meeting the challenges outlined above requires a radical change in the approach to the discovery and development of catalysts, and their wider integration into multifunctional smart devices and materials, as well as production processes. System integration between catalyst, reactor and plant design is necessary.

The potential market impact is (i) an expansion of the uses for catalysts (which may be estimated to be worth about € 2-3 billion, (ii) a reduction in energy or raw material consumption and the avoidance of by-products and waste in chemical processes (worth about € 100-200 billion) and (iii) an improvement in the environment and life quality (worth several billions €).

### Research priorities and roadmap

New research in catalytic transformations should address the following long-term (10-20 years) priorities:

- **Towards 100% selectivity and zero-emission processes.** Design of the next-generation of multifunctional catalysts, by integrating knowledge on hetero-, homo-, single-site and biocatalysts, to achieve 100% selectivity in multi-step and complex syntheses, and to avoid waste formation.
- **Use of non-conventional energy sources.** Exploring new reaction pathways requires a new effort in developing catalysts to be used with non-conventional energy sources (light, electrons, microwave and ultrasound).
- **Use of alternative and/or renewable raw materials.** There is the need for new catalysts for the selective functionalisation of alkanes, gas-to-liquid conversion, and the use of biomass and waste for energy and chemical applications.

- **Catalysis for environment.** New catalysts and catalytic technologies should be directed at reducing greenhouse gas emissions ($CO_2$ conversion to chemicals and fuels, for example), circumventing the breakdown of the ozone layer, and solving water and air issues. Catalysts will also find increasing use in soil and water remediation technologies.
- **Clean energy and mobility**. The development of new and/or more efficient catalytic solutions for clean fuel production are required, meeting the challenge of the widespread use of $H_2$, as well as efficient methods for chemical energy storage and developments to minimise the impact of mobility on the environment.
- **Improving health and quality of life.** New catalysts and catalytic concepts are necessary to address issues, such as indoor and outdoor air quality, purification of drinking water, self-cleaning materials, and catalytic smart sensors.

These long-term objectives require that a series of short-term (5-10 years) objectives are met:

- **Towards tailor-made production of nanoscale materials.** There is the need to develop a new method of synthesis for better, tailor-made control of nanosized catalytic objects and their assembly in a 2D or 3D architecture.
- **Integrate reactor-catalyst-separation design.** Integration and intensification of processes requires the development of new catalytic concepts which break down the current barriers (for example, low flux in catalytic membranes).
- **Develop nanoscale reactors.** Functionalised carbon and metal-oxide nanotubes, new tuneable membranes, novel micro- and mesoporous materials, organic/inorganic hybrids offer breakthrough possibilities for the development of nanoscale reactors in which confinement effects may induce radically new reactivities. Enzyme and microorganisms may be modified to produce or assemble nanoscale catalysts and reactors.
- **Explore unconventional reaction conditions.** It is necessary to intensify the research in unconventional reaction conditions (temperature, pressure, space-velocities), using new clean solvents (ionic liquids, supercritical and $CO_2$ expanded solvents), catalysis with radical and high-energy species (catalysts with non-thermal plasma or radiation, for example), and operations under non-steady-state conditions.
- **Biomimicking catalysts.** Integration of knowledge between single-site, homo-, hetero- and biocatalysis allows for the design of new robust biomimicking catalysts to substitute or integrate with enzymatic and microorganism-driven processes in order to widen their use, reduce sensitivity and increase productivity. New processes for the synthesis of chiral molecules can be developed with these catalysts.
- **Improved methods of understanding of the working of catalysts.** Characterisation of the structure, surface of the active sites during catalytic reaction at the molecular and nanoscale level, understanding the dynamics of transformation, and determination of the nature, mobility and rate of transformation of surface adspecies are some of the challenging problems the solving of which will be the basis for the design of next-generation catalysts.

## Key enablers, linkages, constraints

To turn vision into reality requires a progressive change from search to design in catalytic transformation, discovery and development. The design and implementation for showcase applications must be done in a concerted action between academy and industry. Applications should indicate the direction of research, but the driving force should become the development of new concepts for synthesising catalytic materials, understanding the mechanisms of catalytic transformations and tailoring the assembly of catalytic sites or multi-functionalities in a single site. This change will provide a coherent framework for progress and innovation in catalytic transformations.

*Figure D.3: Catalysis promotes sustainability*[7]

**Promoting a Better Use of Resources**

- Increase of efficiency in the use of energy & resources
- Catalytic upgrading of natural resources
- Use of renewable energy sources
- Reduction of environmental impact of transport

**Promoting Sustainable Processes and Products**

- Eco-efficient catalytic chemical processes
- Gas & liquid emission cleanup
- Conversion of reuse of waste and water
- Reduction of environmental impact of non-chemical processes

**Promoting the Quality of Life and Environment**

- Indoor and outdoor air quality improvement
- Soil and water remediation technologies
- Intelligent mterials / Household user-friendly technologies
- Reduction of greenhouse gases

# 4 Biotechnological Processing

## Challenges

In the past few years, conditions for the application of biotechnological processes in industrial production have improved. New tools, such as screening methods and metabolic engineering, and also global analysis methods, such as genomics, proteomics, metabolomics, and bioinformatics tools, are gradually becoming more widely available. These new instruments make it possible:

- To reduce the time needed to develop and establish new industrial biotechnological products and processes; this was hitherto one of the major drawbacks of biotechnological, as opposed to chemical processes.
- To develop biocatalysts (enzymes) and microorganisms which render manufacturing processes more economical and facilitate new manufacturing processes.
- To apply biotechnological processes with economic potential in the production of basic chemicals and biopolymers.

It is time to intensify, extend and implement this new potential of biotechnological methods in industry so that it can hold its own, both independently and in synergy with chemical processes.

## Scope

In the past, various branches have tended to neglect biotechnological processes in their process planning. Frequently, they are introduced only if serious difficulties arise when implementing individual - mainly chemical - reaction steps in a larger process. However, from the very outset, biotechnology should be included in the decision-making as an alternative to chemical processes. It has the potential to replace several chemical process steps by one enzymatic or fermentation-based production step that is both cost-effective and environmentally-friendly.

This chapter on biotechnological processing focuses on process technology aspects of industrial biotechnology. It is complementary to the *Industrial Biotechnology* chapter and in several cases describes research priorities, which are also mentioned there. It is the aim of this chapter to emphasise that the approaches of chemical reaction & process design and biotechnological reaction & process design comprise many parallel elements and synergies. Both approaches will increasingly supplement each other and become intertwined technologies. Further differentiation between biotechnological processing and industrial biotechnology will be subject to the implementation action plan.

## Vision

Biotechnological processing has the potential to make a considerable contribution towards overcoming the fundamental challenges for industry, namely:

- In the short- to medium-term, by ensuring the competitiveness of European industry. This holds particularly for the chemical industry which, due to the shifting of important markets and fierce worldwide competition, primarily from eastern and southern Asia, is undergoing a phase of reorientation.
- In the medium-term, by improving the sustainability of industrial production.
- In the long-term, by ensuring the exploitation of renewable resources as the primary basis for industrial production and the energy industry, independent of oil.

## Goals - rationale and objectives

Similar to chemistry in the past, it is imperative that biotechnology builds up a pool of methods in order to accelerate the pace of development and implementation. Two examples worth mentioning are DSM's 'plug bug' concept and BASF's enzymatic 'ChiPro' (chiral processes) platform. A combination of genetic engineering methods and analytical high-throughput processes would considerably speed up biocatalyst and process development.

In the past, chemical companies were often hesitant to apply biotechnology. Now however, leading companies have realised its potential and are actively developing biotechnological processes to replace chemical processes, and are also paving the way for new products. Many applications of biotechnological processes in the range of smaller volumes, for example the production of aroma substances, cannot be developed since the achievable volume and margin do not recoup the high R&D expense involved. The advancement of inexpensive and fast methods of strain and process development should therefore be an explicit goal for further research activities.

## Research priorities and roadmap

In the past, when the application of biotechnology was mooted, the chemical industry focused on bioprocesses. In many cases, bioprocesses operate under milder conditions (lower temperatures and pressures, etc.) and are more selective than their chemical counterparts; by these means, bioprocesses conserve resources and improve production processes economically and environmentally. Public debate has often emphasised the advantages for the environment; however, companies are facing hard economic competition, and when a biotechnological process is weighed against a classical chemical process, only the potential economic advantages can affect a shift in favour of biotechnology. Important research areas are:

### Biocatalyst improvement by strain optimisation

At the beginning of the 1990s, as a consequence of the optimisation of whole-cell biocatalysts, the research area of metabolic engineering evolved. This involves the customised improvement of cell properties by modifying or introducing novel biochemical reactions by recombinant DNA techniques.

Undoubtedly the development of production strains for amino acids, vitamins and antibiotics represented a significant milestone in the past. However, it is becoming clear that simple cause-and-effect analysis in biological systems, for example after genetic engineering interventions, is not possible since cell stability, redundancy and homeostasis always cause multiple responses on a genetic, transcriptional and biochemical level.

For this reason, whole-cell biocatalysts have to be investigated holistically; the mechanistic understanding of typical industrial strains must be significantly improved. This can preferentially be achieved by large joint research groups, consisting of microbiologists, (bio)chemists, engineers, (bio)computer scientists and mathematicians. Such systems biology projects can create the requisite knowledge basis for the quantitative determination of the metabolism and hierarchy of cell regulation. This is a prerequisite for tackling interesting biosynthesis paths by deregulation and gene transfer. The result is 'designer bugs'.

Certainly biotechnological process development must be founded on a broader genomic basis. Ten years ago, only a handful of microorganisms with a completely sequenced genome existed; today there are several hundreds. Hitherto priority was given to sequencing pathogenic microorganisms, but it is now high time to sequence microorganisms that are relevant to industry. The following facts show that the potential of a huge number of unknown biocatalysts is still waiting to be tapped:

- Only 1% of the millions of microorganisms that occur naturally are known.
- To date only about 5,000 microorganism strains have been cultivated under laboratory conditions.
- Only 100 microorganism strains have been introduced into approximately 130 industrial processes.

It is therefore of vital interest to sequence more microorganisms. Research in functional genomics should continue unabated, since each sequence has shown that knowledge of the inventory of organisms is indispensable. The aim to define and use a minimum cell inventory for production purposes continues to be a very attractive option.

### New technologies as the basis for novel optimised biocatalysts

A broad genome database provides a foundation for comprehensive microarray analyses (based on oligo or gene chips) to determine intracellular mRNA concentrations and the associated estimate of transcription speeds of all genes of the cell.

Genome data also enable one to decode the proteome of an organism – the total of all proteins present in a cell at a certain time. To investigate the proteome methods for quantitative determination of intracellular protein concentrations, new techniques have been developed (e.g. 2D gel electrophoresis, ICAT/SICAT marker analysis, $^{14}N/^{15}N$ protein quantification), which target the investigation of the cell system as holistically as possible.

Proteins (or more precisely: enzymes) catalyse biochemical reactions using intra-cellular metabolites as reactants. The sum of all reactions and reaction partners is summarised by the terms fluxome and metabolome. Whereas the former has been known in principle through $^{13}C$-based material flow analyses since the mid-nineties, in the past few years increasing efforts have been made to develop techniques for quantitative metabolome analysis (metabolic fingerprinting, metabolic profiling).

These approaches have been supplemented by technological developments, for instance in the area of structure research for pre-calculation of 3D enzyme structures, development of protein-protein interaction cards based on measurement techniques, and *in-vivo* imaging techniques with reporter molecules.

This means that for the first time, extensive measurement techniques are available to determine complex effects quantitatively and holistically. There is every reason to expect that systems biology is a good basis for new process strategies.

### More rapid development and industrial application of biocatalysts – shorter time-to-market

A quantitative understanding of the cell also presupposes the promotion of modelling work in engineering and scientific disciplines. The latter will be in great demand when in the future thermodynamic principles are increasingly applied to the assessment of biotechnological processes (metabolism modelling, downstream processing). Whereas in chemical process development, the integration of thermodynamic issues is a matter of routine, the corresponding biothermodynamic considerations have hitherto been conspicuous by their absence. Especially in the area of downstream processing, a broad, highly complex application area is opening up, which requires intensive input.

Together with the high-throughput screening and selection processes mentioned above, the outcome is a tremendous variety of novel biocatalysts. The activities of BRAIN AG (Germany), and also the example of Diversa (USA), where 100,000 cells are investigated every day and approximately 10,000 (novel) strains are cultivated each month in its GigaMatrix™ system, illustrate how important it is to develop and establish efficient selection and screening processes; these processes should be combined with massively parallel high-throughput techniques for the identification of promising new biocatalysts. The necessary technologies in connection with structure research should be further developed.

This goes hand-in-hand with the need for a high degree of miniaturisation and parallelisation of plant engineering in the framework of microbioprocess engineering.
This explicitly includes downstream processing, which is frequently the main cost factor, although in typical process developments it is often neglected. It is important to develop novel downstream processes for low and high molecular products and to promote techniques which facilitate the effective identification of suitable purification strategies approaches, for example, by improved mechanistic understanding.

### Biocatalyst optimisation by protein design

Tremendous progress has been made in the rapid, tailored development of new enzymatic processes by applying current techniques of directed evolution and genome shuffling, particularly in connection with high-throughput processes for massively parallel analysis of different biocatalysts. These techniques are useful for protein engineering and protein design. The result of such selection and screening processes is optimised enzymes, which can either be used in isolation or in a whole-cell approach as biocatalysts. Here, PCR methods have long facilitated the elucidation of enzymatic activities from extremophile organisms and even from the metagenome. The term metagenome means the sum of the genes of organisms that have hitherto not been cultivable in the laboratory – and that is by far the greater part of the microbial world.

### Bioprocess control and intensification

Optimum control of industrial production processes is still an important matter, which one cannot afford to neglect in the future. Nowadays, modern bioprocesses often use biosensors as online signallers for optimum control. Other novel signals, such as transcriptional or cell morphological signals, could, however, become available for use as new control approaches. Besides the optimisation of control mechanisms, the development of new process and reactor models should be intensified so that the full potential of process control and plant design can be ascertained. Process intensification approaches have by no means been exhausted. Classical bioprocess engineering studies already target the development of process platform technologies for the manifold problems in the area of biotechnology up to technical scale.

### Products

The potential of industrial biotechnology consists in its ability to replace classical chemical production processes and to facilitate the production of new products in combination with chemical catalysis. Products can be fine and speciality chemicals, bulk chemicals and polymers as well as biofuels. It goes without saying that biotechnologically produced goods only have a chance of reaching the market if a biotechnological process makes more economic sense than its competitors. Moreover, the availability of adequate raw materials (especially with the use of renewable resources) for biotechnological processes has to be guaranteed and capacities for recycling residues from biotechnological processes have to be clarified. This includes avoiding unwanted by-products or by-products that cannot be recycled economically.
At present, biotechnological processes tend to be regarded as stand-alone solutions for the production of individual products. For this reason, future processes should aim to build up production networks, to divert by-products to parallel processes and thus to work more economically. One possible approach is to build up biorefineries.

## Key enablers, linkages, constraints

The chemical industry itself developed many of the classical chemical methods it applies today. As for the biotechnological methods, this is rarely the case due to the high development costs, the largely non-existent (but necessary) expertise in the company and the hitherto lengthy development period, at least in SMEs. Here it is often young start-ups that develop the technologies, patent them and even offer them to the chemical industry to use in the framework of various different business models (services, licensing, development partnerships, etc.).
Many young firms and start-ups have adopted the role once held by the central research departments of large-scale chemical companies; this makes for a meaningful development from an economic point of view as it is a means of sharing the burden of high development costs among several companies or several products.

## Financial issues

In some segments biotechnology has already captured a leading market position. The world market volume of prominent product groups, such as amino acids, antibiotics and enzymes, is estimated to be some €55 billion. In 1992, the world market volume of the whole biotechnology branch was approximately €9.6 billion. A selection of highlights follows:

- In recent years, the annual biotechnological production of amino acids exceeded the million ton mark. In vitamin production, there have been several cases lately of a changeover from a chemical to a biotechnological synthetic process, a trend that is expected to increase.
- During the last 10 years, the market volume for enzymes has increased by 50%.
- The successful launching of polylactide marked the industrial biotechnology's breakthrough into the field of polymers and synthetics.

The basis for the successful development of industrial biotechnology is therefore good.

Several studies (BCC[8] Inc., Freedonia[9], and McKinsey & Company[10]) estimate the share of biotechnological processes in the production of various chemical products to be currently around 5%; by 2010, however, they postulate that this figure will raise significantly. For the chemical industry alone, biotechnological production will represent a substantial potential value added. On the one hand, the value added stems from new biotechnological products, and on the other hand from the effects of improved existing manufacturing processes.

The economic advantages, and its clear potential for innovative solutions, show that biotechnological production processes can play a key role in the creation of novel, intelligent products in new production chains.

## 5 Process Intensification

### Challenges

Intensified process equipment and production systems are key enabling factors for step-change improvement in process/plant efficiency, with respect to space, time, energy, raw materials, safety and the environment. Nevertheless, highly intensified process equipment and devices such as micro and/or meso-structured components are, despite substantial development efforts, still reserved to 'niche' areas and have not achieved their true potential on a large-scale in the process industries. Another way to achieve similar objectives is process integration, where operations (such as equipment for heat exchange and mass exchange) are integrated in order to reduce the demand for externally supplied utilities (fuel, electricity, steam, water, solvent, air). The challenge is to identify identical equipment that is the source for utilities and integrate it with operations that are sinks of the same utilities on a plant-wide basis. Future collaborative research must therefore be focused on overcoming the barriers to widespread implementation of process intensification in European industry.

### Scope

New research must cover a much broader range of production scales and production applications, and development must move from individual devices to complete integrated production systems. Widespread application of intensified production requires devices operating under a broad range of conditions, and the development of such devices should be accompanied by a movement toward truly novel synthetic routes for more effective chemical production. Research should address issues both in scale-down for 'ultra' small-scale production of extremely high value-added products early on in the development stages (pharmaceuticals for clinical trials, etc.), as well as scale-up for 'precision engineering' of product end-use properties (such as droplet and grain-size distributions, crystalline polymorphism, isomeric ratios, etc.) for high-tonnage sectors (including polymers, consumer goods, etc.) through locally targeted process control (integrated sensors and actuators). Research should also extend to the impact of new production methods (distributed production, etc.) on safety, plant organisation, supply chain logistics and market response.

### Vision

Robust intensified production systems are an industry standard in Europe, and are available and employed on a routine basis for numerous chemical process applications over a wide range of production scales. They result in improved safety, lower capital expenditure and better use of resources.

### Goals - rationale and objectives

- Development of robust, low-cost, flexible components and systems, including integration of sensors and actuators for locally targeted energy supply and process control.
- Creation of methods, tools and procedures for the widespread use of highly intensified technologies, available and operational at all production scales.
- Innovation beyond individual devices and components through integration of intensified operation into whole-process systems, for true step-change improvement in production and supply chain performance.

#### Mid-term

- **Improving quality and reliability of intensified components and devices.** Research should focus in particular on low-cost fabrication and connection technologies, robust materials, resistance to corrosion and clogging, superior performance with regard to maintenance and reliability for applications under highly demanding temperature and pressure conditions in aggressive and/or unusual media (supercritical fluids, ionic liquids, high temperatures, solvent-free reaction media, etc.).
- **Developing local process control and energy supply.** Priorities involve integrating robust miniaturised sensors and actuators for locally targeted process control, as well as enlarging the scope of process intensification through targeted energy supply for precise control of chemical transformations and reaction pathways, including the use of novel energy sources (e. g. electrochemical, photochemical and microwave devices).

- **Extending processing options for continuous operation.** A major challenge is the invention of methods for the continuous processing of highly viscous and/or solids-containing process fluids in intensified devices, as well as the development of dedicated, small, continuous processes at a reduced cost. A major objective should be a substantial drop in capital expenditure for new plant and/or for retrofit of high-performance intensified devices into existing infrastructure (due for example to operation in much smaller equipment volumes).
- **Process intensification** through integration of heat/mass, reaction/separation, etc.
- **Creating reliable risk and benefit assessment methods.** Among the major issues to be addressed is the creation of new business models for effective, sustainable industrial exploitation of intensified production, as well as criteria for evaluation of safety, reliability and operability of intensified plant.
- **Adapting design procedures, and operational and supply chain management.** Priority should be given to flexible layout and targeted control for integration of intensified components in plant, as well as devising specific virtual prototyping for novel and/or unusual process devices.
- **Identifying the design targets to achieve minimum utility demand.** Priority should be given to flexible layout and targeted control of integration components in plant without sacrificing process operability.

Long-term

- **Adapting intensified process equipment to advances in nanotechnology.** Research should be pluridisciplinary and involve integration into intensified process equipment of nanostructured materials and specifically tailored chemical and biochemical catalysts, enzymatic synthesis, immobilised cell cultures, etc.
- **Implementing self-adapting process devices.** Research in this area should target a new generation of extremely flexible, high-performance process equipment, developed through integration of self-adapting materials (shape-change alloys to create 'intelligent' valves, piezo-electric components, etc.). The long-term goal should be the creation of truly 'programmable' chemical reactors whose local operating conditions adapt automatically to changes in feed composition, product specifications, etc.
- **Creating intensified PRODUCT engineering.** The objective should be to apply process intensification to specifically targeted production of end use properties, including accelerated scale-up methods from bench-top to production scale. The long-term goal should be to combine knowledge of structure-property relationships to define necessary conditions for precise, locally-targeted process control in formulation engineering for rapid response to consumer demand, changing market requirements and mass customisation.

## Key enablers, linkages, constraints

**Enablers:**

- Developments in materials technology and microfabrication methods.
- Improved process modelling and computer-aided design.
- Advances in microfluidics and related disciplines.
- Concurrent process-product engineering.

**Links:**

- New materials: links both for the development of new materials for the process devices themselves, and for the use of intensified processing to produce new products and materials.
- Industrial biotechnology: links to enzymatic and biochemical catalysis, as well as to process intensification involving immobilised cell cultures, genetically modified organisms, etc.

**Constraints:**

- Traditional economies of scale (favouring low-intensity, high-volume operation). For widespread use of intensified process equipment, including the possibility in some cases of distributed and/or delocalised production, a real reduction in required capital investment is a clear constraint for industrial competitiveness.
- Requirement for a new generation of equipment manufacturers capable of producing the required devices and components at low cost. Standardisation is also an issue for interconnection and retrofit.

# 6 In-silico Techniques

## Challenges

If the chemical transformation-based industries are to be globally competitive, catalyst and catalysed processes will have to become evermore efficient and selective. *In-silico* methodologies have become possible through recent technological advances and will have a major impact over the next 20 years. The challenge is to develop *in-silico* techniques (methods and tools) that will enable the design of catalysts, which can be operated and controlled to minimise environmental impact, and yet still achieve significant financial reward. In this respect, aspects of the recovery of valuable chemical products, recycling of unreacted materials and release of inerts or by-products need to be considered in the early stages of the design process.

## Scope

In this section, an opinion is presented of where and what the impact of *in-silico* methodologies might be for the chemical-based industries; however, one must also recognise that other as yet unthought-of developments will also come to pass. Modelling is a core enabler in particular to bridge the gap between the atomistic theoretical understanding and the macro-level process control. Only through the linking of all scales of modelling can one achieve the optimum process and plant configurations.

With the advances of computers and measurement techniques, the possibility to generate and test numerous design alternatives more efficiently and reliably than before is a reality. This means that more new materials can be identified, their application evaluated and their manufacture designed faster and more accurately than before.

## Vision

The recent and accelerating developments in High Performance Computing (HPC), Process Systems Engineering (PSE), Chemical Sensing Technology and Distributed Process Control will ensure that *in-silico* techniques will have a revolutionary impact on the way the chemical industries will operate in the next 20 years. The justification for this point of view is as follows:

- HPC will allow ever more complicated and sophisticated mathematical models to be developed and applied as hardware, costs continue to fall dramatically.
- The dramatic increase in available computing resources allows the application of complex algorithms to become routine even on desktop and handheld PCs.
- Sensor technology is becoming more robust and is moving from confirmation of desired products to control of the delivery of the optimum product yield.
- Miniaturisation of sensors and data transmission devices will facilitate more rapid implementation.
- Web technology and wireless transmission of information will allow the use of distributed computers and integrated distributed process control.
- Powerful and secure communication technology will allow the separation of the location of the process control from the location of the production site.
- Programming methodologies are rapidly developing to exploit the developments in HPC and distributed computing from molecular modelling through cheminformatics to industrial process control.
- Real-time responsiveness will become established in the chemical industries, allowing process steps to be controlled like military aircraft during unsteady state operations, and its effects to be analysed for the whole process for production and purification of the product.

## Goals - rationale and objectives

The ultimate objective of *in-silico* techniques should be the integration of theoretical chemistry, physical chemistry and hydrodynamics at the molecular scale through to the operation of a catalyst at full scale under steady and unsteady state operation. The range of time and length scales that need to be considered is vast, but the integration of currently existing and yet to be developed modelling methodologies will lead to powerful tools allowing definition of an active site, the quantification of the surface chemistry, determination of the rate determining step-through to a rationally based rate equation.

*In-silico* techniques will play an ever-increasing role in all aspects of the chemical industry with the growing requirements of data storage, retrieval, harvesting and mining. With data coming from every step in the industrial process, the area of informatics will become an ever more critical area. In order to articulate these ultimate goals, it is sensible to divide the area into appropriate steps.

### Integrated process simulation

While the application of pharmoinformatics has lead to great advances in all aspects of the drug discovery process, and combinatorial chemistry came with the prerequisite of a means of dealing with all the data, as yet cheminformatics is not widely used within the catalysis industry. The hardware, and much of the software, is available and there is an opportunity now to implement cheminformatics protocols allowing for anyone within a project team, wherever they are in the world, to access all the data from every stage (research, characterisation, development, from scale-up to full plant operation), and have the ability to apply mathematical, statistical, graphical or symbolic methods, which will greatly improve the understanding of chemical information throughout organisations, and will increase the speed-to-market of products.

The use of generic approaches will enable selection from a wide range of methods, building reusable workflows that streamline and even automate analyses, exploiting existing data from legacy applications or on-demand from linked LIMS. As an example, one could consider modelling to optimise experimental conditions when commissioning hardware and to predict the quality of incoming batches by creating a workflow that applies multivariate statistics to each batch to identify regions showing the most variation between batches. This information is then used to optimise the experimental process design and operating.

### Pharmacokinetic simulation (ADME)

Software tools for the assessment of ADME (absorption, distribution, metabolism, and excretion) properties of substances in early stages of the drug R&D process that combine validated mechanistic prediction models with powerful visualisation and selection features, already play a major role in drug discovery, but with the increase in technology described above, the tools will be able to consider ever larger numbers of compounds, with greater accuracy and for greater system complexity. The high-quality estimates of such properties, which have previously only been available from *in-vivo* experiments, are based on elementary physicochemical properties of the compounds. Since these data will more and more be determined *in-vitro* with high-throughput or be predicted *in-silico*, very early rationally-based assessment of ADME behaviour will be possible.

### Biokinetic modelling of chemical plants

Over recent years there has been an increasing trend in measuring and modelling the interaction of contaminants with biological systems at a process level. A typical case is determining the uptake and release kinetics of radionuclides by aquatic organisms, in order to assess the fate of radioactive discharges (past, present and future) in the marine environment.

A variety of biokinetic models already exist and have been used in the design of ideal and non-ideal bioreactors. The effect of the rheology of fermentation broths on mass transfer, mixing, power requirement can be considered, along with residence time distribution analysis as a tool for quantifying non-ideal behaviour.

### Catalyst design

Although High-Throughput Experimentation (HTE) has had a dramatic impact on the development of the latest generation of polymerisation catalysts, this approach has been far less successful in other areas of catalysis. The reason for this failure is the truly enormous range of parameters that have to be explored experimentally. The goal for *in-silico* techniques is to provide first a theoretical direction for the synthesis of new catalytic materials and subsequently to achieve the routine predictive design of catalysts.

### Mechanisms and kinetic models

The majority of homogeneous and heterogeneous catalysed reactions are poorly understood. Consequently, much more rigorous reaction pathways for the desired and undesired chemical transformations have to be clarified. A more accurate theoretically derived definition of the active centre is desirable to fully understand the catalytic cycle. The rate-determining step, and how this is influenced by process variables, can then be inferred. This can only be achieved by close coupling of theoretical and experimental investigations that also take into account heat and molecular transport processes right through the process from reaction to separation and purification. Subsequently, these models can then be used for the development of an integrated and cost-effective health, environment and safety approach towards new processes and plant designs.

## Research priorities and roadmap

- The theoretical modelling of complex homogeneous and heterogeneous systems would have to be significantly developed. The models would have to become much more sophisticated and include things like solvation effects, transition state calculations, etc.
- This would need significant code and HPC hardware implementation, as well as the appropriate protocols for parallel calculations.
- Experimentalists would have to work in much closer collaboration with theoreticians and develop and use characterisation techniques as close as possible to times of reaction transitions.
- Chemical reactions would have to be studied in a much more rigorous way than today to accurately establish the reaction cycles and kinetic models.
- Data mining, optimum selection and integrative analytics will have to be developed for real-time operation research and modelling and simulation fundamentals.
- Further development and validation of models for the complex multiphase systems often encountered in industry, e.g. slurries, bubbly flows, including interphase mass transfer, particle agglomeration and attrition, bubble break-up and coalescence, reaction, etc. This too may require the development of new experimental techniques.
- PSE techniques will be used for designing the process and product together to ensure that products with real potential for manufacture are taken forward.

## Key enablers, linkages, constraints

By their very nature, *in-silico* techniques are intrinsically multidisciplinary and involve multiple length and time scales as well as considering many types of materials and molecules that are traditionally studied in separate sub-disciplines. This means that fundamental methods that were developed in separate contexts need to be combined, and new ones invented. This is the key reason why an alliance of skills from computational chemistry to applied mathematics and computer science will be necessary for the success of theory, modelling and simulation. A new investment in theory, modelling and simulation should facilitate the formation of such alliances and teams of theorists, computational scientists, applied mathematicians and computer scientists.

## 7 Purification and Formulation Engineering

### Challenges

In the final steps of chemical product manufacture, the removal of undesired constituents/features (= purification) and/or the inclusion of additional required constituents/features (= formulation) are the critical steps in meeting customer requirements (e.g. product performance, cost, safety). Societal drivers, such as new legislation regarding product safety and environmental impact, require breakthroughs in this field of technology in order to cope with these future challenges, as well as to remain competitive on a global basis. Significant advances in purification technology and formulation engineering require a much better understanding of the underlying fundamental physics and chemistry on the molecular scale.

### Scope

Tailoring the end use properties of materials by purification and formulation engineering has a broad scope. Separation technology in a broad sense is dominant in purification. However, chemical post-treatment steps (e.g. reactive extrusion of polymers) can be within the scope as well. Improved separation methods with higher selectivities/yields and, especially, less energy consumption are key areas for future R&D. Also novel separation methods for complex molecules (biotechnological, pharmaceutical and food applications) are needed.

Formulation engineering covers a broad field of technologies and applications. For example, in the design of dispersion particulate products, there is a clear trend for particle dimensions to decrease to sub-micron/nanoscale, which will impact new product formulations where surface design is a key factor. Many different fields of applications are covered, e.g. healthcare products, food and consumer products. Also in the field of polymer composites, where nanomaterials need to be dispersed in a homogeneous manner, advances in formulation technology are critical in the development of innovative products.

### Vision

Achieving a paradigm shift in purification and formulation engineering by mastering fundamental chemistry and physics, thus enabling the production of new materials at the lowest possible production cost in zero-emission plants.

### Goals - rationale and objectives

- Replacement of 'mature' separation technologies by new/emerging technologies (e.g. membranes, plasma treatment, electromagnetic or microwave applications, ultra sonic) that will enable lower energy intensity, legislative compliance and improved quality/functionality.
- Mastering the molecular scale in formulation engineering.
- Developing/adapting the necessary technology to account for increased biomaterials and bioprocesses.
- Improved understanding of purification/formulation principles through basic research and modelling fundamentals.

### Research priorities and roadmap

**Mid-term**

- **Separations with alternative sources of fuels and raw materials,** e.g. biomass, fuel cells, clean coal technologies (natural feedstocks, reduce raw materials/energy/climate change/costs).
- **Integrated separations**, e.g. reactive separations, divided wall columns, hybrid processes, etc. (reduce energy/raw materials/cost; also strong link to *Process Intensification*).
- **Separation technology for zero-emission plants and clean products**, e.g. products with zero-residual solvents/monomers and substitution of solvent-based by water-based systems (reduce waste, green chemistry).
- **Formulation of designed products with defined particulate structure**, e.g. micro/nanostructured emulsions and dispersions, dust-free, free flow, hydrophilic/hydrophobic, controlled release, redispersability, etc. (reduce waste/energy/cost; also strong link with *Materials section*).

- **Efficient computer-aided modelling of purification and formulation processes and their sequences**, e.g. automated process synthesis, predictive multi-scale process models with accessible databanks on model parameters (link to *In-Silico* and also *Process Control* and *SCM*).

Long-term

- **Developing the base sciences**, e.g. in affinity, molecular recognition, membranes, but also ongoing fundamental research on crystallisation, chromatography, extraction, adsorption and distillation (link to *Materials* section).
- **New $CO_2$ capture and separation technologies** (reduce climate change).
- **Purification and formulation technology to enable the increased use of biomaterials and bioprocesses** (reduce cost and climate change; strong link to *Industrial Biotechnology* section).
- **Development of perfect mixing**, e.g. enabling the manufacture of new polymer composites.
- **High-purity products by innovative purification/ formulation**, e.g. new medicines and electronic materials, bioproducts from aqueous solutions (link to *Materials* section).
- **Ongoing effort on the development of more environmentally-friendly technology**, e.g. lighter and stronger materials, water purification technology (reduce waste and energy).

### Key enablers, linkages, constraints

Enablers:

- Need for more environmentally-friendly products/ technologies (future legislation, including food safety).
- Coping with higher cost/lower availability of energy and raw materials.
- Increased availability of new materials (e.g. ion exchangers, (affinity)-membranes, solvents, molecular recognition).
- More demanding customer requirements on product functionality/cost/safety.
- Increased collaborative initiatives between industry and academia.

Links:

- To *Materials* and *Industrial Biotechnology* sections, as well as to all other research headings in the *Reaction and Process Design* section. Links to National initiatives, e.g. Dutch Technology Roadmap on Separation Technology[11].

Constraints:

- The European Public/Government underestimates the importance of the chemical industry, resulting in insufficient investment or investment in public research which is too late (e.g. FP6) in this cross-cutting field of technology. Industrial production of chemicals **and** R&D may move out of Europe.

## 8 Plant Control and Supply Chain Management

### Challenges

Chemical process industries provide invaluable base materials for virtually all economic sectors, from food and health to automotive. These industries are sometimes considered to be the 'old economy', traditional, manufacturing products with limited flexibility to adapt to changes in demand. Many of the challenges for industries stem from a lack of understanding and predictability of plant component performance and production processes. This leads to production and market behaviour with limited flexibility, causing sub-optimisation in value chain perspective.

The current state-of-the-art technology still does not permit wide use of real-time, high-quality model-based predictions in the process industries, as models are too costly and too complex. Research has to deliver advanced modelling methodologies, not only for complex continuous flow and batch processes, but also with respect to lifecycle issues. This modelling will enable a step change in process design, operation, maintenance and supply chain management tools that support a new knowledge-based production paradigm and business model for chemical process industries, enabling them to deal proactively with rapidly changing market demands.

### Scope

Novel research approaches need to focus on a breakthrough to generic, low-cost, fast, first principle-based modelling methodology for complex continuous flow and batch processes as well as for lifecycle management. In conjunction with significant research efforts in plant analyser and process control technology as well as novel approaches in plant design and operation, this innovation will deliver next-generation tools for the demanding tasks of:

- Computer-aided process and systems engineering for flexible and intensified processes.
- Advanced process performance monitoring based on intelligent model-based soft sensors and advanced analytical instruments (RMA, NIR).
- High-performance non-linear process control.
- Advanced maintenance and inspection strategies based on models for analysing the plant component state.
- Novel design concepts based on new materials solutions and allowing an extension of the present operation fields of the plants.
- Integrated supply chain management bridging the gap between supply chain network planning, detail scheduling and process design and operations.

### Vision

Production and business paradigm shifts towards knowledge-based, model-centric manufacturing will strongly increase the efficiency and flexibility of the European chemical industry. Advanced plant control, process performance monitoring and supply chain management, as well as progress in lifecycle management will result in flexible, inherently safe production plants with optimal market demand responsiveness.

### Goals – rationale and objective

The target is to push the European chemical industry towards more knowledge-based and customised production and systems organisations through the application of an integrated set of process monitoring and modelling tools, combined with advanced solutions in plant layout for improved performance. Cooperation between industries is vital to learn and share knowledge in order to support the implementation of dynamic manufacturing industries with inter-enterprise operability. In order to achieve these objectives, the incorporation of advances in virtual production, supply chain management and lifecycle management is necessary. This optimisation of the manufacturing processes will facilitate a seamless knowledge information flow along the entire supply chain.

The direct economic benefits mainly consist of expected gains in both cost reduction and turnover increases. Cost reduction results from increased process control and predictability, both in steady state and during state transitions. This will lead to better process efficiency during steady state, shorter transition times and fewer process errors, meaning higher output (+5% to +10%) with significantly lower energy consumption (-5% to -20%), higher plant utilisation (+5% to +20%) and lower waste levels (-25%). Cost reduction will also be generated by optimisation of the inspection and maintenance strategies, as well as by new materials and design solutions. The competitive advantage generated by the ability to produce a greater variety of products at lower cost is expected to create a turnover increase of 10%, thus strengthening the market share of European process industries.

Supply chain costs represent an average of 8-10% of sales revenues for chemical companies. They represent a much higher proportion of the net value added. At roughly 37% of value added in the chemical industry, supply chain costs are significantly more important than in other industrial sectors, such as metal products, building materials, automobiles or paper (where the equivalent percentage ranges from 18 to 30%). This reflects the relatively low value per ton of chemical products and the relatively high costs of moving and storing them, given their bulky and hazardous nature. It also highlights the strong need for supply chain issues to be given high priority in chemical industry.

## Research priorities and roadmap

Meeting the challenges in plant control and flexible manufacturing requires a step change in integrated process and plant operation modelling supported by research in process control systems and process analyser technology, as well as innovative approaches in plant layout. Further to the modelling aspect, the field of supply chain management in the chemical industry calls for significant research work for the development of new methodologies to fully exploit the potential improvement in efficiency and service quality.

The following list contains major research priorities for the respective areas:

### Innovation in process modelling

- Systematic methods and tools for easy and very rapid development of maintainable and consistent lifecycle process models for process and equipment.
- Development and integration of new materials solutions into advanced lifecycle concepts.
- Application-oriented model reduction technologies for the generation of reduced models for real-time optimal plant-wide process operation and predictive control.
- Model-based process monitoring for efficient, reliable and cost-effective process performance monitoring and systems maintenance.
- Closed loop dynamic real-time optimisation even for large scale plants (with multiple production processes).
- Inline asset management determining forecasts for the equipment conditions and effectiveness.
- Supply chain compliant dynamic scheduling.

### Process analyser technology

- From online to inline analyser technology.
- Development of advanced process analyser:
    - Immunoassay analyser for healthcareapplications.
    - Tomographic analyser technology.
    - Innovative magnetic process analyser (e.g. SQUIDS).
- Miniaturisation of process analyser for micro-technology applications.
- Development of new monitoring tools for continuous assessment of plant component state and residual lifetime.

### Supply chain management

- Collaborative planning and control of transport and stock keeping.
- Revenue management.
- Inventories planning under uncertainties.
- Advanced network design for production and distribution systems.
- Reverse logistics – strategies and operational control for the logistics of swaps.

### Key enablers, linkages, constraints

**Enabler:**

- Dynamic development of computational power, development of new sensor principles and innovation in mathematical optimisation routines.

**Links:**

- In the true spirit of supply chain management, particular emphasis has to be placed on collaborative initiatives involving producers, their customers and logistics service providers.

**Constraints:**

- Some of the described innovation challenges will require fundamental changes in business processes, trading practices and managerial mindsets.

# Horizontal Issues

## 1 Introduction

Industry led technology platforms serve the broad interests of EU citizens by facilitating the technological solutions needed to resolve critical societal issues. However, the successful introduction of a new technology often depends on developing an effective public dialogue regarding its costs, risks and benefits and on truly understanding the demand for these benefits. Increasingly the public finds it difficult to cope with the 'unknowns' inherent to new technologies. This often leads to concerns about potential negative impacts of these new technologies. Furthermore, the successful introduction of new technologies also depends in large part on adequate financial resources and on the supply of appropriately trained people. The goal of the Horizontal Issues Group (HIG) is to address these concerns on behalf of all our key stakeholders and to develop a set of priorities that can yield meaningful progress on the above.

The Horizontal Issues Group provides a support function for the overall SusChem vision. In particular the HIG will deliver action programmes that contribute to the earlier and broader societal appreciation of new SusChem technologies, which in turn will foster an increasingly supportive environment for further chemistry-based technological innovations in Europe.

The outputs from the technology areas of the platform and their impact provide the scope for our work. Additional input in terms of both potential benefit and risks also comes from the broader stakeholder groups that make up our HIG network. With an increasing array of issues to address our ability to impact the outcome and the relevance of the issue, SusChem will determine the priorities for the work that will be pursued.

Each of the three *Technology* sections within SusChem has a specific focus as to how their technologies will address issues of major societal importance. These societal drivers are specifically addressed in the SRA. The issues themselves are well known to the public, but what is less well known is how advances in chemistry will contribute to their solution. Chemistry pervades nearly every aspect of manufacturing within the EU, but its overall role is poorly understood for a number of reasons including:

- The benefits of chemistry to essential products are hidden and often inadequately communicated, whereas the risks and potential negative consequences receive frequent media and political attention.
- There is some mistrust of both the industry and the political processes that regulate industry. Indeed, in many European countries there is a distrust of any new technologies that the public find difficult to understand, or where societal concerns have not been addressed during the strategic development of these technologies.

These factors need to be addressed in order for SusChem to provide the technology solutions demanded by our society. This will be how our success is ultimately judged.

## Scope and goals

Scientific and technological excellence play a critical role in innovation, but successful exploitation of innovation also depends on other factors including:

- Aligning the priorities for technology work with the more important market needs, including those relating to consumer acceptance of specific applications in terms of products.
- Increasing access to funding and capital, from both public and private sources.
- Adequately addressing societal concerns, and preferences for technology development in a timely manner.
- Maintaining an appropriate and effective regulatory balance throughout the process.
- Ensuring people with the appropriate skill sets are available to deliver on the above.

The horizontal issues work will include both projects and policy work. By definition the SRA focuses primarily on projects, so the bulk of the horizontal policy work will be integrated into the IAP (Implementation Action Plan) that will follow on from the SRA. SusChem activities will mainly take place within a regulatory framework that is already governed by the REACH legislation; however, by their very nature, new technologies may require new approaches to stakeholder involvement in order for them to be introduced successfully.

The level of interactions from the HIG will range from project proposals and possibly management, to setting up virtual networks and stakeholder dialogue. It will also pursue less resource-intensive actions, such as providing brief position statements on specific issues. Resource priorities will be allocated according to how effectively they can contribute to creating a more supportive environment for our new technologies and make a substantial impact to our stated goals.

Both the pace and global capabilities for technological progress are increasing rapidly. This requires not only that the SusChem technology areas focus on priorities offering global competitive advantage to the EU, but also that the HIG proactively addresses societal concerns and other barriers that might delay beneficial technological progress. Past experience has shown that when delays are based on unfounded concerns, the development of those new technologies simply shifts to other regions in the world.

As well as building early confidence in new technologies, SusChem must also help secure financial support for their development. Industry will of course continue to play a major role in financing research, but better engagement in EU funding programmes and more venture capital initiatives must be sought in order to have a realistic possibility of meeting the societal expectations for the 'enabling industries' that SusChem represents.

The HIG's top level goal is to ensure that the citizens of the EU benefit from the development and use of innovations based on the SusChem SRA. In particular there is a need to ensure that SusChem technologies lead to wealth and job creation for those citizens within the EU, whilst maintaining the high 'quality of life' that we currently enjoy.

## Projects and research priorities

Priority areas for further work within the horizontal arena fit into two themes:

- **Addressing societal concerns** associated with new products and processes. This will involve identification and prioritisation of health, safety, environmental and ethical concerns. From this, effective strategies to disseminate information on risks and benefits as well as the required risk management strategies will be developed.
- **Support for innovation** which involves the evaluation and enhancement of funding models for innovation and processes to develop appropriate skill sets and improve the human capacity for innovation. In addition, different funding options for research and innovation throughout the supply chain will be evaluated, taking into account the needs of the chemistry-based industries, including SMEs.

In the following sections, proposals for projects in the above areas are set out. As SusChem develops an Implementation Action Plan based on the platform SRA, the need for other cross-cutting projects will become apparent. The HIG will identify these needs, evaluate their relative priorities and develop appropriate project proposals to meet them.

In addition a number of other areas for project development, which as yet have not been fully worked upon, have been proposed. They are listed here as an indication of additional areas in which the HIG's efforts may be focused as SusChem refines its priorities for the future. Most of the proposals listed below are in an early stage of development. As SusChem is an open grouping of stakeholders, additional people interested in contributing to these projects are welcome to join. Interested participants should contact the secretariat via our web site – www.suschem.org

## 2 Projects to Enhance SusChem Stakeholder Dialogue

### Facilitating stakeholder dialogue to enhance public understanding of SusChem technologies

**Objectives**

To establish a network of networks encompassing related technology platforms and European activities. This will help improve consumer acceptance for new and emerging (chemistry-based) technologies by harmonising information about their uses, benefits and risks. It is envisaged that this project will be jointly conducted with directorates within the European Commission involved in Research, Enterprise and Communications.

Project deliverables would include:

- Measuring awareness, attitudes and concerns of stakeholders about emerging technologies and their alternatives.
- Developing a global, accessible reference tool that will address these concerns using the most appropriate evidence-based messaging.
- Disseminating the information from the reference tool using appropriate communications strategies.

**Societal drivers**

To sustain its living standards, Europe will need to face up to a multitude of rapidly evolving challenges. With respect to external factors, Europe is disadvantaged versus faster growing regions in terms of access to raw materials and competitive labour costs. It will therefore have to rely increasingly on innovation to compete effectively in the global economy. Other regions are increasing their investments in technologically driven innovations, so a radically improved model for innovation is now urgently needed within Europe for its citizens to maintain their quality of life. These competing regions also typically have a lower risk aversion to change and innovation, which will put Europe at an additional disadvantage if it doesn't succeed in adapting to this speed of technological change. This project will focus on how the successful adoption of novel technologies depends on better addressing stakeholder concerns about the impact of the new technology. Specifically providing information on the risks and benefits of both the novel technologies and realistic alternatives will create a situation in which better informed and more rational choices can be made.

**Rationale**

The contributions of chemistry to developing innovative products and processes, as well as to solving HS&E (Health, Safety & Environmental) problems are often poorly understood. It is therefore important that all stakeholders have access to reliable, valid and objective information. Governments and independent institutions generally have much higher credibility than industry when it comes to communicating the risks and benefits of new technologies. However, for political reasons, critical aspects related to the technology are often not addressed to the public. A more successful innovation model will demand proactive communication of the full facts by credible messengers. This would include better communication on the benefits of new technologies as well as an assessment of how barriers created by slow consumer acceptance would drive the technology innovation to other regions. To make pragmatic progress in addressing such concerns, a number of case studies based on emerging SusChem technologies will be developed. Such studies, in addition to generating factual information, produce a template that can be used to guide future work as well as to develop effective methods for communicating such information. This will ultimately lead to better informed stakeholders and a climate in which optimum decisions representing the majority interests of EU citizens can be taken.

**Methodology**

Desk research will be undertaken to establish what information already exists, to measure awareness, attitudes and concerns of stakeholders about sensitive emerging technologies, such as nanomaterials and the use of genetic engineering to produce crops as sources of energy and feedstocks. This needs to be done for all member states with reference to publications, such as Eurobarometer, to identify those technologies that attract the highest concern in the different member states.

Contact will be made with other existing technology platforms to define cross-cutting issues and overlapping technologies. These platforms' networks would be engaged in the research process.

The project would start with an initial pilot study to refine the issues. This would be followed by a series of workshops in the member states with multiple parties, including national technology organisations, academics, NGOs and government officials. These workshops would address awareness, attitudes and concerns of stakeholders, focusing on knowledge gaps identified in the research about the emerging technologies.

Such workshops would be conducted in member states using the services of a multinational market research organisation. The findings of the survey would prioritise concerns and define the knowledge gaps and misconceptions that need to be addressed to increase consumer acceptance, as critical aspects of SusChem technologies are developed. The information from the workshops will be built into an online reference tool.

**Deliverables**

A joint EU/SusChem/other technology platform-involved report setting out the benefits, uses and risk mitigating strategies will be produced. The content will be tailored to meet the needs of a range of users: technical information for users in the supply chain; overviews of the key issues for decision makers and policy formulators; and non-technical summaries for the wider public and media.

## 3 Projects Improving Risk Management Methodologies

### Integrated testing regimes to support regulatory decision processes

**Objectives**

- Identify and address barriers (time, animal use and resources) to innovation related to regulatory frameworks for future chemical management for the environment governed by REACH within which SusChem will operate.
- To contribute selectively to the EU strategy for the development, promotion, acceptance and application of an Integrated (and intelligent) Testing Framework for regulatory assessment for our new products, that contains as the pivotal principle the concept of reduction, refinement and replacement of experimental animal use. Such an integrated approach is responsive to ongoing EU policy. By focusing on our future technological needs and capabilities, it will also be complementary to the recently launched Alternatives Platform.

**Societal drivers**

REACH is partially a reaction to a societal perception of inadequate chemical risk management. This reaction will also be manifested in concerns surrounding new technologies like nanotechnologies, nanomaterials and biomaterials.

Current regulation of the chemical industry mandates the use of animals to substantiate human and environmental safety of products and services. However, societal acceptance of animal testing is decreasing. In turn, this increases pressure on the need to develop alternative methods without jeopardising safety. Such pressures are reflected in both current and anticipated European policies and regulations (e.g. EU directive 86/609/EEC, the Treaty of Amsterdam and the 7th amendment to the Cosmetics Directive, REACH).

**Rationale**

A science-based process is required to identify and prioritise risk to human health and the environment from chemicals – including novel materials - that optimises the investigation of potential hazards and exposure to determine risk. Such a strategy needs to recognise the need to respect animal welfare and conserve resources.

Prioritisation should be a function of regulatory relevance as well as criteria such as experimental animal numbers consumed and distress/pain. As such it would necessarily include reduction and refinement as well as replacement per se. This necessitates a systematic approach (in contrast to an ad hoc piece-meal approach). There is already sizeable spending, resource commitment and public policy commitment by EU, Member States, NGOs and companies to this issue. The priority for this project is to better integrate these initiatives with a specific focus on our new technologies.

Any search for new strategies must take place in a multi-stakeholder forum that balances (1) the desire of industry and regulators, not to compromise on the protection of humans and the environment (including wildlife), (2) the welfare of laboratory animals as championed by the animal welfare community and shared by all stakeholders, (3) regulatory pressures and (4) economic feasibility.

It will provide an incentive to all stakeholders across the various disciplines and sectors to coordinate efforts and consequently mobilise research and innovation towards achieving the common goal of the 3Rs. Namely, (1) devising new methods that avoid the use of animals while providing meaningful results, (2) developing new or improving existing animal tests so that they provide high-quality information with fewer animals and less suffering and (3) flexible testing regimes that reduce reliance on animal testing.

The EU has both the need and the ability to create capability in this area in response to policy and societal needs. It can work via and leverage existing public and private programmes. There is a need to select useful priorities that are most relevant to the SusChem strategy and to use these to guide future work. Industry will have to deal with a new regulatory framework and therefore needs to be part of the solution. Longer-term sustainability of EU industry will be partially dependent upon acceptance of the concept of Integrated Decision Support Framework (financial feasibility and societal acceptance). The current contribution of industry in this area is poorly understood. Commission technical committees confirm that a research investment strategy driven by a narrow 1R (only reducing animal tests) approach will not deliver the multiple solutions required to address the issue successfully.

### Methodology

Expert workshops will be used to achieve consensus on the use of elements of an Integrated Decision Support Framework with a specific focus on the new SusChem technologies.

The development of an Integrated Decision Support Framework will involve:

- Organising the proper management of identified actions aimed at improving animal testing strategies and the implementation of non-animal strategies where possible.
- Identifying the main research actions needed to meet future regulatory requirements relating to animal use and use of 3R (reducing, refining, replacing animal tests) alternative methods within the chemical industry and other associated industries.
- Identifying the appropriate financial tools required to support identified activities and related coordination actions.
- Gauging the attitudes and concerns of regulators and other stakeholders about the use of an Integrated Decision Support Framework in chemical management.

### Deliverables

A report setting out recommendations about the implementation of a regulatory decision support network for SusChem technologies.

## Intelligent risk management strategies

### Objectives

Continually changing criteria to assess the risks from new technologies, combined with the uncertain impact of environmental factors on human health and the variable application of the 'Precautionary Principle' lead to regulatory uncertainty. This uncertainty creates barriers for innovation and investment. This is true for all three pillars of the SusChem Technology Platform.

The objective of this project is to develop and propose transparent and reliable criteria for an intelligent risk management framework for new technologies. This involves the generation of quality know-how and integrated approaches to give guidance for targeted assessment and management of risks that will serve to reduce the uncertainty to establish public confidence in new solutions.

### Societal Drivers

SusChem Technology Platform implementation will mainly occur in a regulatory environment already governed by REACH. This will make it easier for best practice to be achieved, free of a legacy of concerns associated with current chemicals control legislation. However, this may not be sufficient to address stakeholder concerns about perceived and real potential risks associated with new and emerging technologies.

Unfounded public concerns, often influenced by unqualified views expressed in the media, could lead to inappropriate and unhelpful regulation that does not achieve its objective. It is therefore of vital importance that policies aimed at controlling the risks from new technologies are underpinned by credible scientific information. In order to address the concerns of stakeholders about the ability to control risks from new technologies, an intelligent risk management strategy needs to be developed.

### Rationale

Conventional risk assessment procedures concentrate on data collection rather than on risk reduction. Integration of the relative impact of different risk factors are only rarely used as drivers for action. Along the product lifecycle, several different factors dominate. It is critical to make best use of current knowledge on health impacts and environmental factors in order to get reliable priority driven actions.

To optimise risk reduction, the whole product lifecycle must be examined to identify the points in the supply chain where the greatest exposure to risk exists. The most appropriate intervention points and available control options need to be identified and understood before significant resources are applied to risk management programmes. This approach has the advantage that it can be done in advance of acquiring full toxicological and other data about the hazards and risks of new technologies. This also provides a timely and resource-effective risk reduction tool which can be used to mitigate the effects of new technologies while more extensive data collection continues.

### Methodology

It is proposed that expert workshops be held to:

- Establish the optimum intervention (high-risk) points in product lifecycle/supply chain, illustrated by means of case studies demonstrating good practice that are relevant to SusChem technologies. This should include criteria for dealing with uncertainty in health impacts and priority setting at the health/environment interface.
- Identify knowledge gaps in order to develop intelligent risk management strategies and to underpin regulatory policy with information on exposure mechanisms and control options at the point of use.
- Build on existing work to formulate a common EU approach that industry and regulators can accept and use to develop new screening methodologies and tiered strategies that are based on the 3R concept. This will draw on SusChem networks that will participate in compatible projects. Activities could range from endorsement and promotion of best practices to refining potential research proposals for eventual inclusion and execution within the programme.
- Develop projects that support the themes in FP6 and FP7 in conjunction with ongoing advocacy, expert input and coordination of work related to FP7.
- Define follow-up studies that will further develop and refine risk management strategies.

### Deliverables

The output of this project will be intelligent risk management strategies to reduce the risk from new and emerging SusChem technologies. This will incorporate effective and efficient risk monitoring and management protocols targeted at optimum intervention points in the product lifecycle.

Intelligent risk management strategies will incorporate an in-depth analysis of the implications of risk reduction and control policies. This 'better targeting approach' will also benefit legislations vis-à-vis animal and other resources used for chemical assessment. It will also provide an analysis of the gap of activities necessary to implement an Integrated Decision Support Framework and produce recommendations for appropriate actions to address these needs - an Integrated Decision Support Framework tool kit.

Other outputs will include:

- A support package to provide communications for policy influencers regarding acceptability of an Integrated Decision Support Framework and toolkit.
- Identification of appropriate financial mechanisms required to support identified research activities and related coordination actions.
- Identification of research actions aimed at improving testing strategies.
- Non-competitive FP7 projects that will reduce barriers by addressing generic concerns on regulatory burdens in terms of all resource use.

## Global support for risk assessment techniques in the production of nanomaterials

### Objective

The main aim of this project is to promote wider acceptance of a common global approach for risk assessment techniques and regulations that are being developed for specific SusChem technologies, such as those relating to nanomaterials.

### Societal drivers

The risks associated with key SusChem technologies, such as nanotechnology and aspects of biotechnology, are receiving a lot of media attention. Media attention is often focused on the potential and the perceived risks associated with these technologies and how these have been assessed. This in turn can create confusion and significant consumer concern; hence there is a need to develop globally acceptable approaches to assessing risk in order to gain public confidence.

### Rationale

The number and diversity of initiatives in risk assessment could lead to a fragmented approach to the control of chemical technologies. If inappropriate or contradictory regulations are developed in the EU, it could focus risk management strategies on the wrong priorities. Inappropriate legislation could drive technological innovations and production to other parts of the world. Most importantly, common regulations make best use of limited resources.

### Methodology

Significant resources and public policy commitments have already been made by the EU, individual Member State governments, the US Government, NGOs and industry to develop globally acceptable risk management techniques. SusChem will network with other groups active in this area, such as the ICCA Task Force on Nanotechnology, Cefic's sector group on nanomaterials and other working groups, in order to ensure the development of globally acceptable risk assessment techniques.

SusChem will work via trade associations, learned societies and Member State bodies, as well as leverage output of existing programmes (such as LRI) to develop networks needed to support this project. Member State working groups will be approached to make use of country specific initiatives. Themes that are already being developed within the JRC can be used to contribute to the development of appropriate techniques. Furthermore, the existing work from VCI group can be used to build a common European approach from industry that can be fed into an ICCA endorsed programme.

Industry will need proactively to develop common assessment techniques in close cooperation with credible bodies, such as JRC, EPA METI and OECD.

**Deliverables**

The ultimate output of this project will be the development of globally acceptable risk assessment techniques for SusChem technologies. This will emerge from prioritised 'non-competitive' JRC or Environment projects that will reduce barriers by addressing the generic concerns in areas such as exposure and analytical/control measures.

The first step will be to determine what project areas an EU consortium should tackle on behalf of the global scientific and regulatory community. For example, if the EU focus was on exposure, the following would be included:

- Determine at what points (lifecycle and supply chain) exposures are most likely to pose a risk.
- Identify how exposures can best be measured via globally endorsed methods.

Ultimately, broader societal acceptance issues will need to be supported by multi-level communications aimed at providing information on best practice throughout the supply chain, overviews to inform policy makers, and non-technical summaries for the general public.

## 4 Support for Innovation

**The SusChem support actions for 2005/6 include a specific short-term project to clarify best practices in turning the knowledge from research into productive innovation. This project is likely to stimulate the need for further actions within the framework programme and is therefore included for reference purposes. Potential future research areas under this theme include how to better integrate.**

### Objective

In order to create an optimal environment for innovation, this project will:

- Identify the barriers and promoters of innovation.
- Benchmark European practices against those in the USA, Japan (and possibly other Asian) counterparts to determine best practices.

### Societal drivers

Although Europe is good at creating knowledge, it is poor at turning that knowledge into innovation. For the European chemical industry to remain competitive, this situation will need to improve quickly.

### Rationale

In order to improve the exploitation of innovation, we need to understand the factors underlying the poor translation of European innovation into successful business. It is therefore necessary to review several aspects of the innovation process in order to establish best practice. This project will seek to identify international best practice with regard to:

- Creating financial incentives for start-up companies, including access to venture capital, better access to markets, as well as looking at the roles that fiscal and monetary policy play in stimulating innovation.
- Scientific skills and capacity building needed to support innovation.
- The impact of regulatory frameworks on the innovation process.

### Methodology

Activities include refining potential research topics for eventual inclusion in the programme to capture best practices from other countries or bodies involved in innovation. Both desk research and surveys will be used to compile relevant information. The programme of work will involve:

- A review of existing studies on funding and rewarding innovation, skills capacity building and regulatory frameworks.
- Identification of strengths and weaknesses of different models in relation to SusChem priorities.
- Prioritisation of solutions aimed at enhancing innovation and exploitation of new technologies.

### Deliverables

A report of best international practices with recommendations as to how these could be applied to enhance the successful exploitation of SusChem technologies. This report will serve as an input for the Implementation Action Plan.

## 5 Education, Skills and Capacity Building Projects

### Meeting the skills required by our future industry

**Objective**

The objective of this project is to establish the skills demand in the SusChem technology areas in the short-, medium- and long-term. Having comprehensive information about skills that are required to develop and apply the new technologies, universities and other education and training institutions shall have tools to offer education and training that meets the SusChem needs. The collected information on SusChem needs will also help chemical and biotech companies in their human resources development and life-long learning activities.

**Societal drivers**

There are serious concerns that the number of chemistry and related science graduates across Europe has been in decline for a decade. For example, in Germany numbers fell from a high of over 7,000 graduates per year to around 3,000, although recently, numbers have risen back to around 6,000. However, there are doubts whether these numbers will be maintained. Although less dramatic, falls in the number of chemistry graduates are occurring in most of Europe. The medium- and long-term effect of this decline will impact all areas of research and development in the European chemical industry. Without an adequate supply of appropriately trained researchers, an insufficient quantity of SusChem technologies may be realised within Europe.

In recent years, companies have not signalled substantial recruitment needs. However, when the industry is determined to invest in developing SusChem technologies, researchers and other professionals mastering the new technologies will be needed – and not only in the companies, but also in research institutions.

Life-long learning is an essential part of current working life. This is well understood in the industry. Also, the European Union emphasises the importance of continuous learning as one of the means for achieving the competitiveness goals of Europe. In the chemical industry this means that, as new technologies are introduced, the whole of the workforce continually keeps its skills and knowledge up to date.

**Rationale**

Sustainable chemistry is not a buzz-word, and green chemistry is not just a research item. SusChem is about real cases on eco-friendly products and eco-efficient processes. New technologies will change the skills requirements on all levels, from manufacturing to marketing, research and development, etc. It is essential for the success of the platform to ensure high quality and relevant content of university and vocational education. It should also be kept in mind that researchers and developers of SusChem technologies can have various educational backgrounds, not just chemistry, but also biotechnology, biology, engineering, physics, etc.

In addition to basic education, opportunities for in-service training and further education will be needed. Easy-to-use tools for companies and educators would help developing skills of the workforce.

The aim of this project is to determine what kind of skills will be needed in the chemical industry and research for the development and the application of SusChem technologies. This project will find out whether there is a sufficient supply of appropriately skilled people for the needs of the SusChem technology pillars, and how life-long learning activities in the companies should be developed. Furthermore, this study will determine what needs to be changed in university courses to ensure that the required skills for development of these technologies are taught.

**Methodology**

A survey on the recruitment and skills needs for the chemical industry will be made. In the survey, views of technical, research and human resource managers of identified companies will be studied by means of interviews, questionnaires and case studies.

Questions to be answered in the survey are:

- Numbers working in the field now.
- Recruitment needs now and plans for the future.
- The critical skills needed to develop and apply SusChem technologies.
- How to meet the skills demand now and in the future:
  - By higher education, universities.
  - By vocational education.
  - By human resources development and life-long learning.
  - By offering concrete tools (such as a SusChem database) for educators and companies about:
    - Already existing industrial achievements in SusChem technologies.
    - New technologies and industrial development in progress.
    - Prospects for the future.

This project will be preceded by a fact-finding study mapping ongoing education, training and capacity building initiatives in Europe. The aim of this fact-finding study is to help in designing the survey and to help make decisions on further SusChem actions in education, skills and capacity building. The fact-finding study will also help SusChem to network with other actors in this area.

### Deliverables

- Report on the personnel and skills needs of chemical industry in the SusChem technologies and the ability of university and vocational education to meet these needs.
- Recommendations as to what should be done to meet SusChem's needs.
- [A plan to build] a SusChem database in electronic and paper format.

### Resources and time frame

Estimate of human resources needed for the project:

- Researcher/project manager (part-time).
- [Project manager (part-time) to coordinate/build the database].
- Support group consisting of e.g.:
  - Technical and personnel managers from companies.
  - Professors from chemistry faculties.
  - Experts of vocational training.
  - Representatives from chemical societies.
  - National industry associations.
- Time frame 1-2 years.

## Stimulating the uptake of chemical science courses

### Objective

To support the ongoing national and European initiatives that aim to raise the young people's interest/willingness to choose science and chemistry as their career.

### Societal drivers

Individuals' career preferences are formed at a young age. Even in primary school, children have clear perceptions about industry, science and work in companies and factories. These perceptions have been allowed to decline, but well-planned education-industry cooperation can dramatically reverse this – and later career plans of young people (See e.g. research at CIEC, York[12]). A successful education–industry partnership can only be built if industry is committed to cooperate with teachers and schools. In order to ensure sustainable and successful cooperation, companies must make strategic decisions to be actively involved.

By supporting education-industry partnerships at primary and secondary school levels, SusChem will strengthen the opportunities to get talented young people to choose chemistry, which in turn in the long-term will build the knowledge base and the ability to innovate.

### Rationale

In many European countries, the number of young people choosing chemistry careers has been decreasing for a long time. Reasons for this development are diverse. The negative image of chemistry and the general downward trends in the number of students taking the natural sciences in higher education may partly explain the trends, but additionally the reduced career opportunities in the chemical companies, academia and the public sector may play a part. Nonetheless, as SusChem aims to build the knowledge base and raise the level of innovation of the chemical industry, a continuous supply of talented young people choosing careers in chemistry is essential for the success of the platform.

Numerous projects have been initiated on local, national and European levels to reverse the trend. Many scientific, industrial and other organisations and SusChem stakeholder groups are working actively in this field. As SusChem would clearly benefit from the success of these projects, the platform's support for these projects is entirely appropriate.

### Methodology

A survey of major European and national projects aiming at developing the young peoples'/children's understanding of chemistry as a crucial contributor in our everyday life, and perceptions about the chemical industry and research as an interesting career should be undertaken.

Based on the results of the survey, an assessment will be made of how SusChem can add value to these activities.

### Deliverables

- A SusChem position paper on the importance of education and industry partnerships.
- Closer involvement in on-going projects, if such involvement is seen to add value to SusChem.
- The use of specific SusChem networks to make such partnerships easier to manage.

Time frame priority: to be started in 1-2 years.

# 6 Lifecycle Assessment Processes

## An EU endorsed approach to lifecycle assessment (LCA)

### Objectives

We aim at the mid- to long-term goal of advancing the Lifecycle Thinking (LCT) and practice for integrated and holistic environmental and sustainability assessment of products, processes and services in the EU. This will be achieved by assembling a critical mass of data and expertise and by creating a momentum amongst the participants and stakeholders. The main purpose of the proposed activity under this Technology Platform would be to foster 'lifecycle thinking' through a much more widespread data collection, data exchange, technical development, dissemination and use of LCA and related tools. By fostering lifecycle thinking in areas relevant to the SusChem technologies, the LCA project will support and complement the other suggested projects 'Intelligent Risk Management Strategies' and - to some extent – 'Global Support for Risk Assessment Techniques' by broadening the range of environmental relevant topics to be included in the evaluation of SusChem technologies beyond risk-based considerations. Most importantly, more widespread use of LCT will enable a wider range of stakeholders to make better informed decisions about the true impact of our new technologies.

### Societal drivers

LCT is gaining more and more ground and LCA is expected by many to become a pivotal tool for a holistic environmental and sustainability assessment of products, processes and services in the EU (e.g. in the context of the management of finite natural resources, basing eco-design more on facts rather than fashion and making better use of our solid waste).

### Rationale

The efforts will build on and be linked into existing, 'horizontal', functional expertise networks (e.g. the United Nations Environment Programme/Society for Environmental Toxicology and Chemistry (UNEP/SETAC) Lifecycle Initiative, the OMNIITOX project and the efforts at the JRC, Ispra, to create a European platform for quality assured data for LCA). However, the active participation of industrial stakeholders in the UNEP/SETAC Lifecycle Initiative for example has remained somewhat lower than expected. Thus, the main new element of the activities will be the strong 'vertical' integration of current and new LCA stakeholders along the industrial 'design-production-service-end-of-life' value chain with strong industry representation.

The expected benefits of such a multi-dimensional structure will be piloted in a few selected sectors to enable more reliable and complete data collection and exchange, education and dissemination of learning for all stakeholders, including SMEs. This integration will allow both the optimisation of the lifecycle of industrial systems, products and services, and the practical implementation of new industrial solutions based on lifecycle thinking.

### Methodology

Within the proposed activities, the interaction with two bodies with distinct function is envisaged:

- A European LCA Research Council consisting of all relevant stakeholders from governments, academia, NGOs and industry to optimise research efforts in a complementary, multi-disciplinary way. Here, a close cooperation with the Lifecycle Assessment Steering Committee of SETAC Europe will be established.
- A Multi-Stakeholder Study Cell for providing the authorities with independent scientific and technical perspective for use of LCA in EU policy making.

Furthermore, several discussion groups (web-based) and workshops (web-based and face-to-face) will be established to facilitate the work on:

- Harmonisation of Lifecycle Inventory (LCI) data documentation formats: With the aim to enhance compatibility and applicability of LCI data from different data sources, these efforts will go beyond the existing technical specifications in the ISO framework (ISO/TS 14048 Data documentation format), e.g. by building on the best practice development in the UNEP/SETAC LC initiative and the ongoing efforts at the JRC, Ispra, to create a European platform for quality assured data for LCA. The work should support and complement the current efforts of the European Commission by also addressing questions of appropriate data quality, data quality indicators, measures of quantifying or at least estimating uncertainties for LCI data, building on expertise from relevant industrial players along the supply chain.
- LCA data gathering: Based on agreed data documentation formats, web-based tools will be established to enhance a sustained contribution of the network to the collection of harmonised LCI and LCA data relevant to the SusChem SRA activities. Again, these efforts will support and complement the current efforts at the JRC, Ispra, to create a European platform containing harmonised LCI datasets on some key materials and processes.

Other key elements of the planned work are communication and training aspects:

- 'Grandfathering' and pioneering new vertical links of networks by attracting and defining common projects with 'Associated Partners' within and outside the EU, along the cradle-to-grave chain. Larger industrial companies with LCA experience would offer training and case study opportunities to SMEs.
- Coordinating and planning LCA education sessions, trainings and workshops (cf. SETAC LCA workshops), an organised student exchange programme.
- Input and dissemination of acquired data and knowledge via the ongoing efforts to create a European platform on LCA tools and data and via the UNEP/SETAC Lifecycle Initiative and other national and regional platforms.

## Deliverables

The vertical axis of the project will drive implementation and dissemination via demonstration or pilot studies on lifecycle assessment approaches and best practice in different industrial sectors:

- Creation and dissemination of reliable and accepted data and information tools on SusChem technologies using widely applicable formats.
- Creation of a multi-stakeholder study cell for policy advice.
- Coordination and avoidance of duplication of research work. Overall contribution to sustainable development by applying holistic and quantitative tools.

Expected benefits for governments, industry and consumers that translate lifecycle thinking into practice will consist of:

- Institutionalising lifecycle thinking in EU industry and consumers, with a strong vertical axis down the value chain.
- Ensuring a better understanding of the environmental issues at stake in the context of the SusChem technologies by all stakeholders, from a more holistic environmental perspective.
- Strengthening the cooperation between companies along the value chain and stakeholders from governments and e.g. consumer organisations.
- Ensuring applicability and dissemination in the EU, but also more globally, e.g. via UNEP/SETAC.

## 7 Linkages to FP7 Programmes

An important role for SusChem, particularly for SMEs with limited resources, is to facilitate the identification of potential sources of project funding. Technology driven projects will mainly focus on cooperative research. This is the area consuming the bulk of the FP7 programme. The themes most relevant to chemistry, and also the area where the bulk of the SusChem resources will be targeted, are already described in the second section of the *Synergies* chapter in the SRA. The HIG will examine relevant funding options for projects that are more driven by societal concerns. Here the focus will be on different themes or indeed other programmes, such as the examples illustrated in Table E.1.

*Table E.1: FP7 programmes related to activities of horizontal issues work*

| Programme | Theme | Sub-theme | Horizontal linkage |
|---|---|---|---|
| Cooperation | Energy | Knowledge for energy policy making | Societal & competitivity issues of alternative feedstocks |
| | Environment | Climate change | Main solutions via technology areas. Some impact via renewables |
| | | Environmental technologies | Developments in product modelling and exposure assessments |
| | Socio-economic | Growth, employment & competitiveness | Potential projects following benchmark study |
| | | Combining economic, social & environment | Communication and risk management issues |
| | | Trends in society | Acceptability of emerging biotechnology and nanotechnology |
| | | Europe in the world | Coordinated approach to potential regulatory processes for emerging biotechnology and nanotechnology |
| | | Socio-economic and scientific indicators | Fact based communications |
| People | Lifelong training | | Multi-disciplinary needs |
| | Industry-academia pathways | | Potential projects following benchmark study |
| Capacities | Research for SMEs | Research for SMEs | Chemistry specific potential project in definition phase |
| | | SME assistance via networks (via CIP) | Chemistry specific potential project in definition phase |
| | Science in society | Improving EU science system | Need to clarify scope and role for SusChem |
| | | Science and technology and their place in society | Societal concerns for emerging technologies |
| | | Improved communication | Communication and risk management-issues |
| JRC | JRC (non nuclear) | | Intelligent risk assessment |
| | | | Global coordination contributions |

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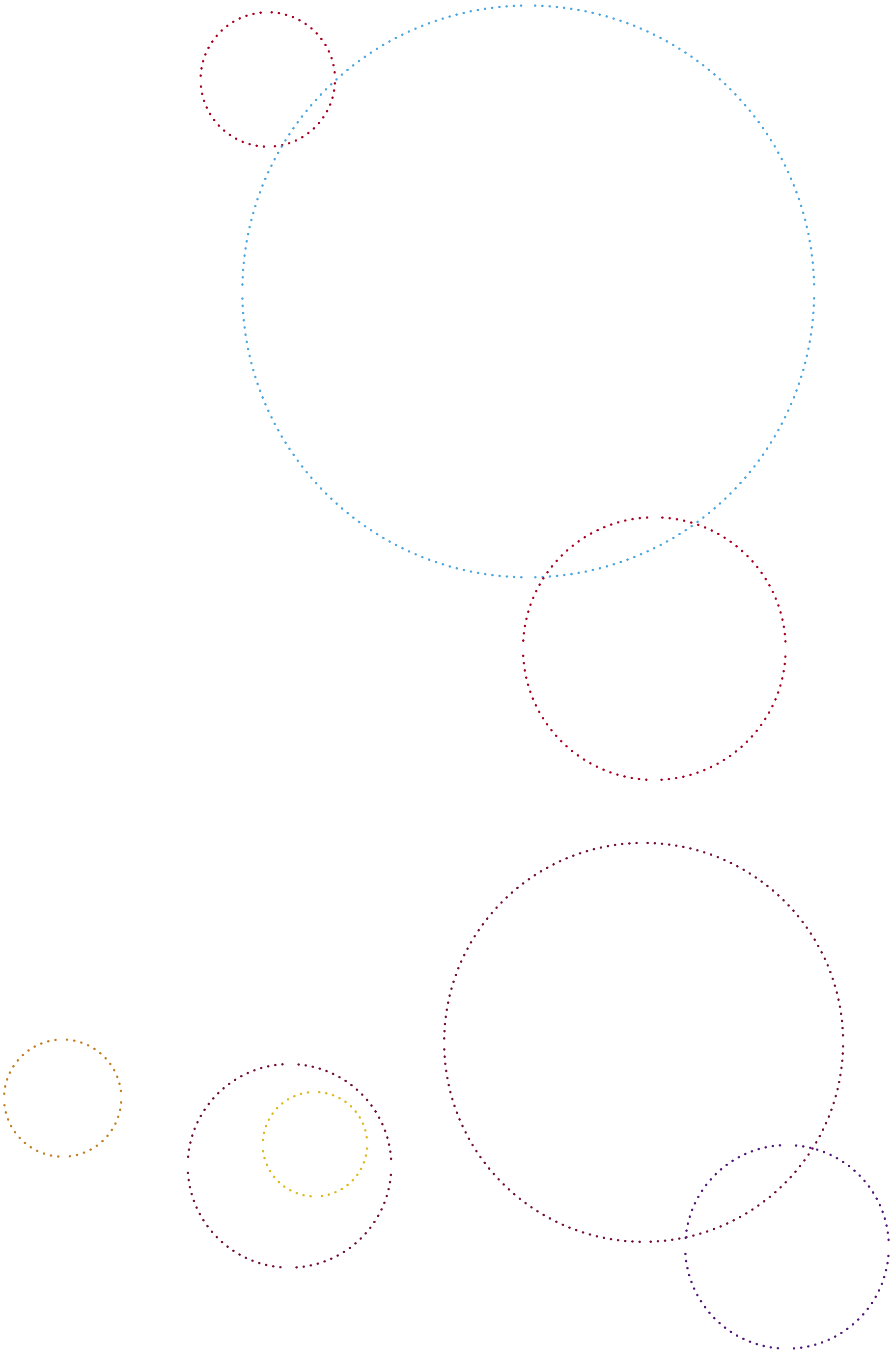

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