SusChem
European Technology Platform For
SUSTAINABLE CHEMISTRY

SusChem IAP Update 2009

Reaction & Process Design

1 Reaction & Process Design IAP Update

1.1 Introduction

The SusChem Reaction & Process Design (R&PD) Core Group, chaired by Dr. Klaus Sommer of Bayer Technology Services, Germany, consists of European experts in topics related to reaction and process technologies such as synthetic chemistry, catalysis, reaction engineering, purification and formulation engineering, process modelling and simulation, process intensification, plant control and supply chain management. The group has been responsible for the R&PD content of the SusChem Strategic Research Agenda (SRA) and the respective contributions to the Implementation Action Plan (IAP). In the latter document, R&PD topics are in par-ticular represented in the chapter "Sustainable product and process design".

Since the finalisation of the SRA and IAP documents, the group has been reviewing and assessing the take-up of R&PD topics in the FP7 work programmes. Subsequently, the group's work has been focussed on recommendations for future calls based on this assessment.

The group acknowledges that R&PD topics have been well represented in the FP7 calls in 2007 and 2008, in particular in the NMP work programme, and also with biotechnology and biomass related topics in the FAB and Energy programmes. The group notes that SusChem research priorities addressing different R&PD aspects have often been combined and aggregated in these calls. While this seems reasonable from an impact point of view, this approach leads to a broader scope for calls and might have invited substantial oversubscription to the calls. In some cases, designated long-term research priorities have been addressed in the early calls (e.g. "programmable chemical reactors" in "Process intensification in chemicals production"), and it might have been too early to effectively target these research fields with projects. The group recommends that the subscription rates and quality of proposals in those areas, where many research fields have been combined, be carefully assessed and, based on this assessment, subsequent additional calls in these areas be considered.

The group further proposes to strengthen multidisciplinary approaches for process intensifica-tion projects. This should be explicitly included in respective calls. For ambitious projects in this area social sciences and economics might be included as disciplines beyond the usual research and technology developments, to get products/research outcomes that have clear economic and sustainable potential. This could potentially be a research topic in itself.

More dedicated work is needed on process understanding. For instance, in PAT (Process Analytical Technology) too much emphasis is put on analytical tools rather than in developing a rationale on what should be measured, what the best approach to measurement is and how this leads to a better process understanding. Current US strategies of the National Institute for Pharmaceutical Technology and Education address the same aspects of knowledge-based pharmaceutical product/process design.

In addition, through a joint effort between SusChem, the European Technology Platform on Water Sanitation and Supply (WssTP), and other stakeholders from the Chemical Industry, a new area of research focusing on Integrated Water Management and Industrial Water Use has been addressed. The results of this collaborative exercise and a list of research topics are presented in section 1.2.9.

1.2 Recommendations for IAP update and future FP7 calls

1.2.1 Materials handling in intensified process systems

As the chemistry-using industries begin to adopt process design approaches enabling appro-priate use of intensified process strategies then the limiting factors controlling process performance cease to be equipment-oriented and tend towards the process materials themselves. In pharmaceutical and fine chemicals manufacture many processes involve solids either as feedstock, intermediates or final effect products. Equipment with small scales of structure are not ideally suited to processes using solids, and if additional solvent use is required to process otherwise solid reagents in small scale systems then some of the benefits of intensification are negated. Processes involving viscous liquids, gels and foams are equally common, and have their own difficulties to address to successfully implement intensified processing.

1.2.1.1 Relation to SusChem IAP

This topic is an extension of key activity "Advanced product engineering" in the IAP chapter "Sustainable product and process design". The original key activity and its extension comprise key technology developments for sustainable chemical manufacturing.

1.2.1.2 FP7 Uptake of this topic

Continuous processing of highly viscous and/ or solids-containing process fluids in intensified devices was addressed as one of numerous elements in the call for small/medium scale projects NMP-2007-3.2-2 "Process intensification in chemicals production". As the key activity tackles major technological hurdles this has not been sufficiently covered by this call.

1.2.1.3 Gaps

- Standard methods of characterising materials behaviour, particularly with respect to composition/make-up and its effect.
- Multiscale understanding of materials behaviour, application to process design.
- New equipment types.

1.2.1.4 R&D objectives

- Development of materials characterisation techniques
- Development of methodologies to understand materials behaviour, collation of generic results for common systems, application to real processes at multiple length scales
- Identification of opportunities for new intensive equipment types suited to solid/viscous liquid/gel/foam processes, prototype development and testing

1.2.1.5 Recommendation

Address this topic with a research oriented call for small/ medium scale projects or a large call including demo activities for intensified product engineering addressing the challenges of the topic.

1.2.2 Fostering the industrial take-up of electrochemical synthesis

As a specifically targeted energy source, electricity as an activator for physical and chemical transformations should offer substantial advantages in terms of precision control, selectivity process performance and energy savings.

1.2.2.1 Relation to SusChem IAP

This topic is related to key activity "New synthetic pathways" in the chapter "Sustainable product and process design", but has only implicitly been mentioned as utilisation of electrons as alternative energy option in catalytic pathways.

1.2.2.2 FP7 Uptake of this topic

The topic has not been mentioned explicitly in any calls so far. However, it could have been addressed in principal in the two calls on synthetic pathways: NMP-2007-3.4-2 Innovative pathways in synthesis and NMP-2009-3.2-1 Innovative pathways for sustainable chemical production.

1.2.2.3 Gaps

The focus of further R&D activities should be on suitable reactor design rather than research on reactions, as the latter has been exhaustively investigated without related industrial response.

1.2.2.4 R&D objectives

- Substitution, via electrochemical reactions, of traditional oxidising and reducing agents
- Selective, atom-efficient electrochemical synthesis routes
- Electrochemical methods for local control of chemical composition and field strength in processes for product formulation: powder production, agglomeration, phase formation, particle and droplet size distributions
- Electrochemical surface functionalisation
- Segmentedelectrochemical surface functionalisation
- segmented and structured reactors for electro-organic synthesis, including specific local control of electrocatalytic activity
- Electrochemically assisted bioenzymatic transformations
- Integration of new materials, new catalysts and new promising synthesis routes in electrochemical processes
- More efficient energy integration and recovery in electrochemical processes
- Electrolysis for hydrogen production (including high-temperature electrolysis)

1.2.2.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects.

1.2.3 Alternative forms of energy for new chemistries, new synthetic routes, new products and Process Intensification

Alternative sources and forms of energy, such as electromagnetic, electric, acoustic or high-gravity fields have been shown to be able to modify chemical reaction paths and to deliver new functional products with properties not achievable with conventional technologies. Many of those energy forms can intensify chemical and biochemical processes with effects exceeding two or even three orders of magnitude.

Alternative forms and transfer mechanisms of energy may also significantly enlarge the applicability potential of micro-structured reactors via:

- Accelerating chemical processes to "fit" in Microsystems.
- Reaching higher product yields by combining alternative energy transfer mechanisms with microprocessing features (e.g. fast heating-up of the reactants and a fast quenching of the products).
- Reducing or preventing some basic problems in the microprocessing system operation, such as fouling.

1.2.3.1 Relation to SusChem IAP

This topic is an extension of key activity "Reduction of resources and waste" in which the development of clean intensified processes using unconventional forms and sources of energy has already been mentioned.

1.2.3.2 FP7 Uptake of this topic

The topic has not been addressed in any calls. It has been on the list of indicative future topics for NMP for some time.

1.2.3.3 Gaps

- The basic engineering understanding of the mechanisms behind the alternative energy-based processes and of the relationships between various parameters influencing those processes is still insufficient.
- In order to apply more alternative sources and forms of energy on a commercial scale, a more intensive multidisciplinary research effort in those areas is needed. Close research collaboration between chemical engineering and other disciplines, chemistry, materials science, electronics and applied physics in particular, will be of crucial importance here.

1.2.3.4 R&D objectives

- Research on basic engineering concepts of alternative energy-based processes
- Particular products which are difficult to obtain using conventional processing methods.
- Methods for targeted supply of innovative forms of energy including reactor concepts for precise control of chemical transformations and reaction pathways
- Use for novel reactions to yield new products with unique functionalities

1.2.3.5 Recommendation

Address this topic with a research oriented call for small/medium scale projects.

1.2.4 Innovation challenges in formulation engineering

Formulation of products is a widespread and diverse activity in the chemical-using industries that suffers many manufacturing problems associated with difficulties on process design, scale-up and lack of robustness. There are several global markets reliant on the science of formulation, their combined value is of in the order of thousands of billions of US dollars (USD) per annum. A few examples are: European Pharmaceutical market stood at USD 337 billion in 1999 with EU having 26.6% share (IMS World Review 2000); Crop protection market, global value USD 23 billion (Syngenta Crop Protection Regional and Country Detail November 2006); Personal care, USD 21 billion for Procter & Gamble alone (P&G annual report 2007). Accessing even moderate savings, through "quality by design", reduced development time, lower energy consumption, improved efficiency, and lower rejects rates, in just a small percentage of these markets has the potential to provide savings of hundreds of millions USD per annum.

1.2.4.1 Relation to SusChem IAP

This topic builds on key activity "Advanced product engineering" in the chapter "Sustainable product and process design", but suggests a more holistic and systematic approach to product engineering.

1.2.4.2 FP7 Uptake of this topic

Several aspects have been addressed in NMP-2007-3.2-2 "Process Intensification in chemicals production", but only as part of a highly diverse call for small/medium sized projects. The NMP 2010 call foresees a call on "High throughput technologies for the development of formulated products"

1.2.4.3 Gaps

Although there is scientific understanding of specific types of physical and chemical phenomena relating to formulation at individual length scales, creating and stabilising a formulation in a manufacturing plant involves multiple physical interactions taking place simultaneously at many different length scales. Understanding of these combined effects, how they impact on product quality and process robustness, and how they may be manipulated and controlled to improve product quality and process robustness, is currently limited and not trivial. Technical and scientific capability and competence is a big issue and Corporate knowledge on formulation is difficult to retain and retrieve because much "know how" is experiential and empirical.

1.2.4.4 R&D objectives

- Development of whole process methodologies/tools based on fundamental understanding of mapping the formulated product characteristics to process and product performance and then linking these characteristics to the underlying chemistry and physics at various length scales (bulk, particulate, molecular) that take place during manufacturing and storage
- Development of experimental and theoretical techniques to verify the underlying chemistry and physics
- Application of the above tools to define the necessary work/decision flows for efficient and effective formulation process development and implementation
- Demonstration of application of the above tools for the characterisation of intrinsic manufacturability to guide formulation development in the determination of appropriate programmes of experimental work and in the rapid identification of robust process options
- Development of methods and techniques, based on fundamental understanding, which stabilise freshly produced nanoparticles (primary particles) without influencing their surface functionality or properties

1.2.4.5 Recommendation

The importance and required critical mass of this topic warrants a call for large scale projects.

1.2.5 Membrane-based hybrid separation or chemical conversion

Until now, membrane technology has not been part of the standard toolbox of process designers and engineers in the process industry.

1.2.5.1 Relation to SusChem IAP

Membrane separation is partially addressed in IAP chapter "Biobased Economy" as an "innovative downstream process", and in the chapter "Sustainable product and process design" as "in situ product removal in bioreactive separations". In the same chapter, integrated reactive and hybrid separations are a dedicated topic of key activity "reduction of resources and waste".

1.2.5.2 FP7 Uptake of this topic

Downstream processing has been generally neglected in the FP7 calls so far. Membrane separations have been addressed only in the area of water purification, in NMP-2009-2.6-1 "Novel membranes for water technologies".

1.2.5.3 Gaps

In general, membrane technology is not a proven technology and large-scale introduction of membrane processes, despite their potential advantages, is hampered by lack of:

- A good membrane material selection process for the operation window required for a given application. Aspects of such a process include membrane flux, selectivity, stability/lifetime issues in relation to high temperature/pressure operation, solvent resistance, pH window, fouling, etc.
- Standardisation of design rules and engineering solutions for modules (i.e. sealing and surface-to-volume ratio, cleaning, replacement strategies) and system concepts
- Shared experiences with promising applications in terms of costs and profits, test results, operational reliability, etc.
- Successful results from large-scale applications

1.2.5.4 R&D objectives

Application areas that could benefit from membrane technology and require substantial R&D effort include:

- Upfront separation of olefins and paraffins to simplify distillation separations to carbon number separations alone
- Fischer-Tropsch: removal of water, downstream of reactor
- Equilibrium-limited reactions: methane steam reforming, including water gas shift. Removal of H_2, CO and/or CO_2, preferably in the reactor
- Ammonia or methanol synthesis: product removal, either in the synthesis reactor or downstream
- Alkane (ethane, propane) dehydrogenation: removal of hydrogen in the reactor with/without hydrogen oxidation
- Alcohol (ethanol, tert. butanol) dehydration: removal of water in the reactor
- Oxidation reactions: Provide oxygen-enriched air, provide a controlled amount of O_2 through a membrane for safety or higher selectivity
- Industrial biotechnology applications: product removal to prevent inhibition or water removal in work-up

1.2.5.5 Recommendation

Address this topic in the NMP area with a research-oriented call for small/medium scale projects or a large call including demonstration activities.

1.2.6 Multiscale modelling and modelling of complex systems

The development of mathematical models for representation of the domain process/product knowledge is still principally a manual task. A significant reduction in time and resources spent on in-silico research in general, and modelling in particular, can be made through the development and use of cyber modelling frameworks. These can aid in the systematic generation/creation of the needed models, which is usually the first-step of any model-based approach. A versatile and flexible modelling framework with features such as model reuse, model decomposition and model aggregation coupled with advanced software architectures, plug & play with models and software integration will be able to promote significant advances, not only in the area of in-silico research, but in all other research/applications dependent on models.

1.2.6.1 Relation to SusChem IAP

In-silico techniques are partially addressed in IAP chapter "Sustainable product and process design" as "computer-added design methods and tools", however strong emphasis is put on equipment design and process optimisation aspects. A dedicated effort on multiscale modelling as described above is missing.

1.2.6.2 FP7 Uptake of this topic

No dedicated call has been issued on this topic.

1.2.6.3 Gaps

A major challenge is the modelling of complex systems and systems representing different scales. This is a prerequisite for process modelling tools meeting the needs of current process technology directions.

1.2.6.4 R&D objectives

- Development of a library of predictive constitutive models with the capability to generate the necessary models of different scales of size, form and application for a wide range of problems at a fraction of the time and resources spent currently
- Systematic fitting of models to experimental data including model structure discrimination and model-base experimental design; flexible and generic framework (architecture) for a computer aided modelling system useable by all disciplines
- Development of 'Plug & Play' models from various sources and of various sizes

Emphasis could also be given to the efficient use of models – that is, how to obtain innovative solutions from model based solution approaches. If the model is simply used to replace the experiment, while some savings in time can be achieved, it is doubtful if innovative solutions can be found.

1.2.6.5 Recommendation

Generally, modelling aspects have been considered as part of the toolbox in different calls of the production theme in NMP, but a dedicated call targeting the required software advances is probably out of the scope for NMP alone. Therefore a dedicated joint ICT-NMP call is recommended.

1.2.7 Process monitoring and control in intensified process systems

In contrast to large petrochemical processes, many fine chemical and pharmaceutical production processes are not optimised, resulting in decreased capacity utilisation (10-20%) and a portion of the end-product falling outside specification (10-20%). Costs of non-optimised production amount to 1-2% of total turnover. Reasons to maintain non-optimised production include:

- Unknown fluctuations in raw material quality (e.g. seasonal effects, different suppliers, variations in composition of intermediate chemicals production processes)
- The absence of an adequate physico-chemical model describing the relationship between process parameters and product quality
- The suboptimal design and control of processes

Robust monitoring and control of processes is critical to the successful deployment of intensified process technologies. The adoption of appropriately scaled intensive equipment enables precise control over localised process conditions. Precise control encourages the use of less stable regimes (e.g. higher temperatures and concentrations, operating inside the explosion limit), which also demands more from process monitoring and control instruments/systems.

Process Analytical Technology (PAT) is seen as best practice philosophy in pharmaceutical and fine chemicals manufacture, but fundamental process understanding is important to identify the critical process parameters requiring monitoring and control before thinking about measurement solutions.

1.2.7.1 Relation to SusChem IAP

This topic is an extension of the area "Miniaturised sensors and inline analyser technology" in the chapter on "Sustainable product and process design".

1.2.7.2 FP7 Uptake of this topic

No dedicated call has been issued on this topic.

1.2.7.3 Gaps

- A methodological approach to identifying and selecting critical process parameters for control in reaction, isolation and product formulation processes.
- Robust sensors for measurement of a variety of defined critical process parameters in microscale equipment and process systems.

1.2.7.4 R&D objectives

- Development of methodological approaches to the identification and selection of critical process parameters requiring control in reaction, isolation and formulation processes
- Development of sensor technologies capable of measuring defined critical process parameters in microscale equipment and process systems
- New and improved sensor techniques. Fast, accurate and robust online sensors are needed to determine whether products are within specification and whether processes are running optimally. This can enable the transition from batch to continuous processing.
- Many parameters that determine product composition can not currently be measured online: colour, turbidity, taste, odour, low concentrations of reactants and intermediates and microbiological components (contaminants like penicillin, viruses and pesticides). To this end, completely new sensor techniques need to be developed.
- In addition, the amount of information obtained from standard techniques could be much improved by more sophisticated signal analysis techniques.

1.2.7.5 Recommendation

A dedicated NMP call on process monitoring and control and development of miniaturised sensors.

1.2.8 Sustainability of whole process systems

The concept of sustainability is becoming increasingly important in the chemistry-using industries but often carries differing definitions between different business areas and/or different organisations. All will agree that the overall objective is to develop and operate economically viable processes with minimal impact on the environment and the population in terms of raw material use, energy use and waste. This requires metrics for sustainability assessment, which integrate the examination of costs, environmental impact and social effects of different product or process alternatives in the search for socio-eco-efficient solutions.

1.2.8.1 Relation to SusChem IAP

This topic emphasises the area "Lifecycle Analysis" in the IAP chapter on "Sustainable product and process design".

1.2.8.2 FP7 Uptake of this topic

No dedicated call has been issued on this topic.

1.2.8.3 Gaps

Metrics are available to assess the sustainability of processes in terms of either economic or environmental impacts, though none assess both economic and environmental impacts together. No current sustainability metrics address societal impacts. Yet together these three factors are the key drivers on which sustainability decisions are made by industry.

1.2.8.4 R&D objectives

- Use of existing sustainability metrics to quantify sustainable performance, and development of appropriate metrics for areas not currently covered
- Methodologies to develop and implement sustainable process plant – e.g. plant layout for minimal energy use in multi-purpose batch and/or intensified/multi-scale facilities, selection of cleaning versus disposable/biodegradable process equipment
- Methodologies to enable appropriate selection of sustainable process technologies for a given manufacturing process when assessed against economic, environmental and societal drivers

1.2.8.5 Recommendation

A strong requirement for sustainability/lifecycle assessment is recommended for projects, which claim the development of more sustainable solutions. In addition, the further development and harmonisation of sustainability assessment tools should be facilitated.

1.2.9 Integrated water management and industrial water use

Society demands an increased focus on the sustainable use of water. There is an ongoing competition for water between agriculture, urban areas and industry, which will grow stronger over the coming years, taking societal mega-trends into account. To become more independent from the issue of scarcity of water, there is an industrial need for more integrated use of water to ensure reliability of supply.

The European Frame Work Directive demands a higher quality of surface water for the coming years, less influenced by industrial use of water or by industrial products and thus further driving this competition forward.

In a joint effort between the European Technology Platforms SusChem and Water Sanitation and Supply (WssTP), including inputs from the Chemical Industry, a list of topics for collaborations have been identified.

1.2.9.1 Relation to SusChem IAP

This topic comprises a new field of activities going beyond the original SusChem IAP, in which "(bio)catalytic solutions for water remediation and purification of drinking water" have been promoted in the chapter on "Quality of Life".

1.2.9.2 FP7 Uptake of this topic

Water is one of the key areas under the activities "Sustainable Management of Resources" and "Environmental Technologies" of the Environment Work Programme. NMP issued the call NMP-2009-2.6-1 "Novel membranes for water technologies" in 2009.

1.2.9.3 Gaps

The water industry needs for its research and technology development:

- New chemical products such as new separation compounds with less environmental impact, optimised dosing, more selective reaction
- New materials, e.g. reactive membranes, corrosion resistant units, bio film inhibiting
- The exchange of information to transfer innovative concepts in process engineering e.g. like separation, monitoring or control technologies

The chemical and process industry needs to integrate routes that:

- Allow for less impacts, in particular on water resources, by minimising consumption, optimising recovery by new syntheses, and considering water recycling as part of its operation
- Decrease the vulnerability of water consuming processes
- Secure supply especially under the threat of Climate Change

1.2.9.4 R&D objectives

High priority topics include:

- Define and implement demonstrations of best practices in integrated water management systems for the 2020 water footprint of chemical industry operations in typical geographic diverse locations
  - Case studies on cooperation between process industries and other actors involved in water/wastewater management on a river basin scale. Analysis of the case study, boundary conditions, problems, solutions. Specifying demand for development of interfaces between different sectors, e.g. industrial, municipal, agricultural.
  - Case studies should cover cooperation projects, e.g. in a costal region, an inland region and an example of cooperation with SME/medium size process industry plants. Preference should be given to case studies

in river basins that already face a severe water stress according to the water exploitation index (WEI).

- Process efficiency of water use, addressing also the related energy aspects and possible relationship to bio-based platform chemicals and biorefineries
- Process efficiency
  - In cooling/heating processes, by using innovative processes and technologies (e.g. micro heat exchanger) and linkage with improved production processes
  - In water demand within production processes using water as carrier
  - In processes having water as part of the product
  - In efficient use of water treatment chemicals (e.g. to minimise membrane fouling, to treat recalcitrant compounds)
- Increasing energy efficiency of water treatment in process industry, including both process water and wastewater treatment.
  - Balancing water - energy demands and production
  - More cost effective processes by extracting energy from industrial (heat) rejects and wastes
  - Recovery of valuable resources, e.g. low heat energy from wastewater, recovery of substances (e.g. carbon in form of biopolymers (PHA), process catalysts, valuable trace elements etc)
  - More cost and energy efficient treatment of highly loaded liquid streams (e.g. process and wastewater)
- Provision of water treatment technologies in bio-energy production, future production of bio-based platform chemicals and operation of biorefineries. Development of clean biofuel plants and biorefineries down to the zero-waste objective.
- Provide efficient treatment technologies for Priority Substances and emerging pollutants
- Closing of the water cycle, and defining optimal limits of closure. Reuse of water on a local scale (plant) and regional scale such as integrated management of water resources, inter-actions between municipal, industrial and agricultural use (reuse and cascade use of water).
- Development of coDevelop a co-operation with working groups tasked with the revision of the BREF (Best Available Techniques Reference) documents
- Bring together experts from process industries and water industries to integrate routes
  - To allow for minimising water and energy consumption
  - For increasing water and energy recovery
  - To allow conversion of valuable compounds within wastewater into energy and products, and
  - For considering water recycling as part of their design and operation
- Drive the developments of enhanced materials, process technologies and systems
  - Bring together experts from process industries and water industries to create innovative solutions for water and energy efficient technologies and for more flexible water treatment processes
  - New materials
    - To increase performance of e.g. separation technologies (e.g. membranes)
    - To reduce corrosion, fouling, generation of biofilms
    - Functionalised for water treatment
  - New treatment concepts (e.g. new technologies or innovative combination of technologies/systems) for new production methods in process industry
  - Cross developments e.g. application transfer from process industry to water treatment, application transfer across different process industries, et cetera

1.2.9.5 Recommendation

Strong uptake by the environmental programme, including the consideration of joint calls with NMP

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