STW programma:

Green & Smart Process Technologies

26 oktober 2006

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CONTENT

1. Executive Summary

In view of the high relevance (in terms of annual turnover, contribution to gross national product, and employment) of the chemical process industry for the Dutch economy, STW has decided to start a STW seed programme named ‘Green & Smart Process Technologies’ (GSPT).

GSPT should contribute and enhance the competitiveness of this branch of industry as well as boost and strengthen the position of the process technology groups at the Dutch universities of technology.

GSPT aims at revisiting the choices for process routes and/or reactors, usually made decennia ago under different boundary conditions with respect to sustainability, economy and state of the art in catalysis and other chemical engineering fields, and to try and come up with more sustainable alternatives.

GSPT aims at breakthroughs resulting in reductions by a factor 2 to 5 in

- the consumption of energy, mineral deposits and other raw materials,
- the production of CO_2 and other environmental loads,
- safety risks, and
- investments and operating costs of plants

GSPT is about drastic changes in reactor engineering technologies, about step-outs outdating familiar concepts such as unit operations and scale-up rules. A great leap forward toward reaching the goal of a more sustainable world requires a tremendous effort from the engineering community: a large number of power generation and production processes are in need of a fundamental review. GSPT is not only about developing more sustainable process alternatives as such, but particularly concerns applying them on an industrial scale economically viably.

The three themes eligible for support within GSPT are *process architecture*, *process intensification* and enabling technologies. In this way, GSPT intends to generate new leads for industry to radically improve chemical processes and plants in terms of energy use and cost/benefit ratio.

The research projects carried out under the umbrella of the GSPT Programme should be multi-disciplinary, process technology taking the lead, with contributions from such divergent fields as micro-system technology, industrial catalysis, chemistry, thermodynamics, materials science, transport phenomena, computational techniques and process control.

The technology developed at the universities should be transferred to industry or alternatively offer opportunities for new companies. Knowledge exchange between industry and academia is stimulated from the start of the research projects. GSPT should create a basis for a strong patent position for the participating Dutch companies.

The success of GSPT depends on the extent to which a fruitful interaction and collaboration is realized between the various (technological) fields participating in the envisaged multi-disciplinary research projects. The multi-disciplinary approach makes GSPT different from other research programmes such as PoaC, IBOS, BBASIC and ASPECT; furthermore, the time horizon of GSPT is shorter. It is anticipated that GSPT paves the way for a larger and longer-term research initiative of the type of DSTI.

2. Ambition of the Programme 'Green & Smart Process Technologies'

The STW Programme 'Green & Smart Process Technologies' (GSPT) aims at:

- developing breakthrough technologies with impact on science and industry in a time frame of 4 up to 8 years, among other things by providing a basis for a strong patent position for the participating Dutch companies
- generating new leads for industry to radically improve chemical processes and plants in terms of energy use and cost/benefit ratio
- drastic changes in reactor engineering technologies, comprising step-outs outdating familiar concepts such as unit operations and scale-up rules
- contributing to the developments of a more sustainable and competitive process industry in the Netherlands and Europe
- encouraging the process technology groups at the Dutch (technical) universities to explore new leads and ideas in the core field of reactor engineering

The research projects carried out under the umbrella of the GSPT Programme should be multi-disciplinary, process technology taking the lead, with contributions from such divergent fields as micro-system technology, industrial catalysis, chemistry, thermodynamics, materials science, computational techniques and process control.

3. Relevance of GSPT for the Netherlands

The chemical sector plays an essential role in the Dutch economy. The annual turnover amounts to some 40 billion euros and makes up about 3% of the gross national product. Some 70,000 people are directly employed within the sector in more than 500 companies. It is estimated that the sector including supplies, transport, infrastructural investments and high level services, accounts for 10% of the total industrial labour force and takes care of some 20% of the Dutch export value.

Worldwide, the Dutch chemical sector is one of the leaders in base chemicals, food ingredients, coatings and high performance materials. Location, physical and knowledge infrastructure, availability of feedstock and strong innovative companies form the pillars of this successful cluster. Europe-wide, the chemical sector has taken initiative by developing a Strategic Research Agenda emphasising the importance of strengthening its position and innovation potential.

In the Netherlands, the 'Regiegroep Chemie' [1] has recently published an ambitious plan to further strengthen the position of this sector and aims at doubling its contribution to the gross national product within 10 years and to halve the use of fossil feedstock in 25 years. Essential for this ambition is a world-class position of technical competences in the field of industrial biotechnology, catalysis engineering, materials and process technology. The STW Seed Programme GSPT fits into this ambition and is a translation of it in the field of process technology. It embodies a breakthrough multi-disciplinary systems approach to innovative processes and process equipment, by integrating the competences of the various process technology research groups at the Dutch (technical) universities.

[1] http://www.vnci.nl

3.1. A surroundings analysis

Europe's chemical industry Although Europe has still a very strong and leading position as being world's largest chemicals producer, exporter, importer, and consumer [2], surely the chemical industry has to focus on maintaining this position in a very competitive world by considerably strengthening it's innovative power and increasing its R&D investments. Only in this way Europe's chemical industry may maintain its strong position at the centre of technological innovation (see also [3]).

Dutch chemical industry Dutch industry finds itself in a very competitive global environment, where economic strength is determined by having the best technologies available and by social geography. Production cost reduction and control is and will remain an important driver. Furthermore, legal constraints ('license to operate') will become increasingly important in the short run. This holds for the existing as well as new production arenas. In view of long-term competitiveness, it is essential for the Dutch chemical industry to be able to manufacture new materials with new functionalities, while the energy requirement of production should be reduced dramatically or change to different sources, capital costs for new equipment being low.

In view of these drivers, industry is seeking process improvements and breakthrough technologies through a stronger integration of disciplines, which is guided by an integrated approach to academic development. Especially in the Dutch context only few such programmes are available, *e.g.* bio-products (BBASIC), fine (bio)chemicals (IBOS) and separations (DSTI). These programmes have limited focus on improving current commercial chemical reactions and processes, and will provide solutions between 10-15 years from now. It is, however, of utmost importance that, next to these structures, a research programme is available, which has the chemical reactor as the centre and realizes breakthrough technologies and processes by integrating developments from different research areas into highly improved manufacturing systems (equipment and processes).

Foresight scenario This strong position relies amongst others on the availability and further development of innovative process equipment. Finally this should lead to real-life applications and implementation in industry, which should be among the guiding principles in defining the focus and scope of R&D programmes. Recent trends in process intensification and micro technology open challenging horizons to equipment innovation, enabling new manufacturing and processing methods. This has led to appealing and challenging foresight scenario's in which it is envisaged that future leading European process technology will be based on a wide-spread implementation and use of intensified, high-precision process equipment and devices, including corresponding adaptation of plant management, supply chain organization, and business models [3, 4].

IChemE The foresight scenario developed by the (British) Institution of Chemical Engineers (IChemE, [4]) sketches a world that will only require small numbers of chemical engineers to design and operate oil refineries, petrochemical plants, and similar "traditional" large-scale continuous processes. According to IChemE, chemical process industry in North America and Europe will move towards "effect products" and manufacturers will have not only to produce more sustainably, but also to deploy the most advanced product science and technology. This will require chemical engineering research to move to the forefront of advanced materials synthesis and manufacturing technologies in order to retain competitive edge. Being the first in this development will create big opportunities. This appealing future of chemical engineering as sketched by IChemE and others is basic to the GSPT programme.

Chemical Engineering in the Netherlands A large part of the GSPT programme will be carried out at Dutch universities, in particular, as may be envisaged, at the universities of technology, where the majority of the chemical engineering groups are located. Over the last years, the academic position of the field of chemical engineering in the Netherlands has weakened, albeit still a number of excellent and internationally renowned groups demonstrate a strong impact (as, for example, illustrated by the recently founded Dutch Separation Technologies Institute, DSTI). This weakened position is a result of the continuously decreasing number of students, a number of departmental reorganizations, the actual closing-down of research groups and their facilities, and the discontinuation of certain research activities.

Clearly, this GSPT programme will provide the opportunity to boost the research activities in the field of chemical engineering in an innovative field of research with large importance for the chemical industry as well. This provides challenging opportunities for collaboration between university groups with different expertises leading to a multidisciplinary approach in which chemical engineering disciplines will tie up with expert groups providing enabling technologies.

[2.] E. Croufer, The Staying Power of Europe's Chemical Industry, Prism, 1, 2005, pp. 29-43.
[3.] K. Sommer, Strategic Research Agenda – Reaction and Process Design, SusChem, European Platform for Sustainable Chemistry, 3rd Stakeholder Meeting, London, November 25, 2005.
[4.] Institute of Chemical Engineers (IChemE), United Kingdom (http://foresight.ichem.org).

3.2. Current developments in Process Technology

For several decades, chemical process industry was dominated by the "economy of scale" paradigm. Nowadays, it becomes clear that achieving the goals of sustainability not only requires new chemistries and new products, but also requires fundamental changes in the chemical routes and processing methods for manufacturing those products. This is a 'communis opinio' in the world of the chemical process industries and has been worded at several occasions, as for example in the Green Manifesto of the Netherlands Research School in Process Technology OSPT [5a,5b].

> *The need of concerted research efforts in the field of green process technology may best be illustrated by the increased rate of melting of the Arctic Ice. To mitigate the negative effects of the current manufacturing processes on our Earth, its atmosphere and climate, and its finite resources of clean air, clean water, forests, fossil fuels and ores, big steps are needed in developing more sustainable manufacturing processes.*

Revisiting our current methods of manufacturing the whole range of energy carriers, base and fine chemicals, food and pharmaceuticals is necessary and urgent. This research programme Green & Smart Process Technologies (GSPT) responds to this development.

Developments of the past few years show the rapidly increasing importance of GSPT, both in the Netherlands and abroad. GSPT comprises and combines a number of recent novel approaches and concepts. The most important of them are Green (Sustainable) Chemistry, Process Intensification (PI), Microreactor Technology, and Chain Efficiency.

In the Netherlands, PI has been recognized as an important element of the key-area "Chemistry" by the Innovation Platform. The Chain Efficiency Platform of the Energy Transition programme has recently recognized PI as a promising route to substantial energy savings in Dutch chemical, pharmaceutical and food industries over the next 50 years.

On the international arena, GSPT-like developments were reported on several international symposia and conferences such as the International Conference on Sustainable (Bio)Chemical Process Technology (Delft, September 2005) and the 1st International IUPAC Conference on Green-Sustainable Chemistry (Dresden, September 2006). In 2005, the European Federation of Chemical Engineering established the Working Party on Process Intensification. This new Working Party, among other things, collaborates closely with the European Technology Platform on Sustainable Chemistry (SUSCHEM) to bring PI subjects into the 7th Framework Programme of the European Union.

Next to all the R&D activities, first commercial applications of the intensified "Green Smart Manufacturing" technologies have already taken place. Examples here are the micro-processing units implemented in the production environment by such companies as Merck, DSM and Clariant.

[5a] Van den Akker H.E.A. (2001), Groene Manifest: op weg naar een groene procestechnologie, NPT Procestechnologie 8 (5) 5-6
[5b] Franken A.A.J.M. (2005), Duurzame 'groene' procestechnologie, NPT Procestechnologie 12 (5) 7

3.3. Opportunities for value creation

The potential impact of the programme in terms of value creation for the society as a whole, for the sector, for mechanical and mechatronic manufacturing industries, the supply sector, engineering and consulting services directly and via spin-off / spin-out activities is very significant.

It will contribute to value creation in various ways (depending on the type of processes) such as:

- Improvement of long-term competitiveness through enhanced process knowledge and higher quality and/or new products; selectivity and yield increases by application of these technologies up to 10 times may be expected; a decrease in by-product formation up to 75%
- Improvement of major cost factors by reduced energy use (20 – 80%) and reduced capital investments (20 – 80%); direct energy savings are expected to be significant in all sectors of the process industry. A conservative estimate for the Netherlands amounts to 25 to 45 PJ/a in 2030 representing a value of 250 to 500 M€ /a (2005)
- Significant increase in process safety resulting from a significant decrease in reactor volume and inventory of intermediates (10-1000 times) and better reaction control
- The paradigm shift from 'economy of scale' to 'economy of numbers' may open vast opportunities for new business models and other playing fields in which high-tech SME's due to relatively smaller capital needs and risks per case may play an import role
- Opportunities for extended retrofit of existing plants may lead to complete new process possibilities
- Diminishing time needed for product and process development and for market introduction
- Enabling distributed processing thereby changing the whole chain and reducing the need for transportation
- Enhanced adaptability to changing business environment by increased flexibility in using *e.g.* different feed stocks
- Enabling distributed processing thereby changing the whole chain and reducing the need of transportation (saving fuel, risk reduction)
- New markets for equipment and service vendors
- Cross industry sector synergy, *e.g.* between chemical and food processing industry or (analytical/control) equipment manufacturing industry
- New opportunities for equipment and service vendors in existing and new markets
- Improvement of the image of the sector
- Education of skilled high-level labour force

3.4. Recent trends in the field of chemical engineering

Innovation in reactor engineering New reactor engineering options and solutions are foreseen as the result of the continuous quest for better and intensified processes with considerably improved energy and process efficiencies and economics. Challenging concepts are proposed such as multi-purpose, self-adapting, and modular process devices using advanced sensor and process analyser technologies and programmable chemical reactors whose local operating conditions adapt automatically to changes in feed composition and product specifications [2].

Incentives and drivers for change Specific incentives for introduction of these new equipment technologies are for example market flexibility with shorter delivery times, use of locally produced raw materials, decentralised and continuous manufacturing, lessened risk with the transport of dangerous materials, improved product properties, and just-in-time and on-demand production closer to the end-user (consumer or industry). These developments may even lead to business models in which chemicals manufactures become technology service and systems providers. Of course, these developments will strongly impact on the nature and scale of process equipment, pilot plants, and production devices, and therefore may even change the chemical industry's skyline.

The economic drivers for introducing these technologies are obviously the result of the continuous focus of the chemical industries on substantial reductions in capital expenditure through lower investment and operational costs, lower energy needs, and reduction of emissions (such as CO_2). The targets for costs reduction may vary for different types of chemical industries and are related to the type of processing, the production capacity, and the product portfolio, but should certainly be of the order of more than 50% to be reached after a period of 10 to 15 year. These targets can not be met by the existing industrial and academic research and development programmes. The gap between the present and new technologies can only be overcome through a major investment in R&D.

Collaboration between industry and academia A strong private-public collaboration and a close interaction between industry and academia are definite prerequisites for a successful development and implementation of these new technologies and business models. Obviously, this requires new national and European research initiatives that focus on a multidisciplinary approach and integration of various technologies in long-term and coherent R&D programmes [3, 6, 7].

So far, in the Netherlands no such initiatives are foreseen, which illustrates the urgency of this GSPT programme in order to link up with related ongoing and new developments in Europe (in particular Germany) and in the USA and in Japan [7,8]. In Germany, six Fraunhofer institutes have created the 'Fraunhofer Alliance for Modular Microreaction Systems' (FAMOS, [9]). Other organizations include the 'New Jersey Center for Micro-Chemical Systems' (NJCMCS, [10]) in the USA and the MicroChemical Process Technology Research Association in Japan (MCPT, [11]). All these research institutes and organisations have a strong participation of industry.

Faster and cheaper process design Throughout the chemical industry, a uniform desire is to make process scale-up and design faster and cheaper. However, full-scale designs must be robust and of high quality. The process systems and control area traditionally deals with the design and operation of processing plants. Novel processing concepts need to be translated into conceptual process designs that can be flexibly operated in a much more sustainable way. Options should be explored for replacing current types of reactors by more 'green' alternatives. A major goal in reactor system selection, design and scale-up is to reduce the number of development steps used to move from concept to production facility, *e.g.* by eliminating pilot plants owing to the exploitation of advanced CFD, and to reduce the so-called time to market.

Process Safety Industry is responding to developments within a society that struggles with growing concerns as to safety. Accidents such as those in Three Miles Island, Seveso, Bhopal, Enschede, Toulouse and London turned safety into an issue in the public debate; companies should earn a 'licence to operate'. Such a licence is pretty relevant in modern societies in which mature citizens are very critical about industrial activity in general and chemistry and chemical industry in particular, and about their impact on health, safety and environment.

Reduction of Transport Flows The synthesis of fuels and chemicals in large industrial complexes leads to huge material flows worldwide. These material flows represent a heavy burden for the transport infrastructure. Reduction of material transport is therefore highly relevant. In the transport of chemicals, transportation safety may be an issue as well: some chemicals present a hazard due to their toxic or flammable nature. Reduction of materials transport could be brought about by, among other things, decentralised synthesis of intermediate of final products at the end-user. This involves scale-down of synthesis facilities rather than scale-up.

Recycling and Closing of Materials and Energy Loops Extensive product flows tend to create extensive waste flows. Our modern society suffers from enormous transport flows of metals, paper, biomass, fuel and polymers. Within the sector of chemical process technology, the conversion of biomass based products and that of polymer based products need to be tackled. One of the options is to convert these materials back to new raw materials. A second option is the conversion of waste materials into preferably transportable fuels.

[6.] Netherlands Organisation for Scientific Research, Chemicals Sciences Division, 'Strategische koers voor de chemie 2007-2010', The Hague, The Netherlands, June 2006.
[7.] Jaarverslag Technologiestichting STW, Utrecht, The Netherlands, 2005.
[8.] A.M. Thayer, Harnessing Microreactions, Cover Story, Chemical & Engineering News, 83 (22), 2005, pp. 43-52; http://pubs.acs.org/cen/coverstory/83/8322finechemicals.html
[9.] FAMOS; http://www.mikroreaktionstechnik.info/
[10.] NJCMCS; http://www.njcmcs.org/
[11.] MCPT; http://www.mcpt.jp/eindex.html

3.5. Summary

GSPT is a STW Seed Programme and is intended to take the lead in a process of re-strengthening and restructuring the position of the process technology groups at the Dutch universities. Building on the internationally renowned strengths of a number of existing research groups and fostering the development of new lines of research should guarantee the sustained viability of this important Dutch discipline. By doing so, it should provide a stimulus to Dutch universities for maintaining a knowledge base and a suitable infrastructure in important science fields involved in the development of novel process and manufacturing methods for chemical compounds.

In addition, this programme intends to generate new leads for industry to radically improve chemical processes and plants in terms of energy use and cost/benefit ratio. This programme aims at contributing to the development of a more sustainable and more competitive industry in the Netherlands and Europe and must enhance the capability of the Dutch industry to create and exploit new processes. The research projects should result in breakthrough technologies with impact on science and industry in a timeframe of 4 up to 8 years.

The technology developed at the universities should be transferred to industry or alternatively offer opportunities for new companies. Knowledge exchange between industry and academia is stimulated from the start of the research projects.

The ambition of the GSPT programme is to come up with a number of patents that is larger than the average in STW projects along the complete technology field (usual is one patent per 2 M€ granted and an exploitation level of 60%) providing a basis for a strong patent position for the Dutch companies involved. Further results of the GSPT programme should comprise an improved knowledge infrastructure, a strengthened know-how position of the research groups involved, and a contribution to the start up of a larger innovation programme in the Netherlands or Europe.

4. Research themes in GSPT

The ambitions mentioned in Chapter 1 of this document have been translated into a number of concrete targets which may best be pursued by focusing on a limited number of research themes. These targets and themes will be highlighted briefly in this Chapter 3.

4.1. The targets of GSPT

GSPT aims at revisiting the choices for process routes and reactors, usually made decennia ago under different boundary conditions with respect to sustainability, economy and state of the art in catalysis and other chemical engineering fields, and to try and come up with alternative, more sustainable alternatives. This process is already going on in industry – though at a low pace.

GSPT aims at breakthroughs resulting in reductions by a factor 2 to 5 in

- the consumption of energy, mineral deposits and other raw materials,
- the production of CO_2 and other environmental loads,
- safety risks, and
- investments and operating costs of plants

Further characteristics of GSPT relate to reduction of waste streams (by-products), with re-using waste or auxiliaries within the process itself, and with avoiding the use of inflammable, toxic or carcinogenic compounds as intermediate products or auxiliaries. In addition – and this is the key issue of this proposal - complete processes and plants have to be re-designed in order to meet novel 'green' standards.

4.2. GSPT in a nutshell

GSPT is about drastic changes in reactor engineering technologies, about step-outs outdating familiar concepts such as unit operations and scale-up rules. A great leap forward toward reaching the goal of a more sustainable world requires a tremendous effort from the engineering community: a large number of power generation and production processes are in need of a fundamental review. GSPT is not only about developing more sustainable process alternatives as such, but particularly concerns applying them on an industrial scale economically viably.

A non-exhausting list of examples of how such drastic changes could be attained, comprises

- finding novel process routes requiring *e.g.* different, 'greener' reactants, more active and more selective catalysts, 'greener' solvents, milder operating conditions and/or avoiding nasty by-products;
- integration of several process steps, *e.g.* multiple reaction steps in cascade synthesis reactors;
- optimisation of reactor geometries and operating conditions *via* computational simulations;
- use of micro reactors;
- Process Intensification;
- making processes more flexible in term of raw materials use, by means of sophisticated process control, eliminating *e.g.* the need of extensive raw materials blending

GSPT focuses on two themes only, *viz.* novel process architectures and process intensification. Research in the fields of these two themes may greatly be facilitated by recent advances in computer technology, simulation capabilities and process synthesis. That is why within GSPT also support can be given as to the development of so-called enabling technologies. The three themes eligible for support within GSPT are therefore *process architecture*, *process intensification* and enabling technologies; these three themes will now be introduced briefly. Potential applicants are referred to Annex 1 in which a more extensive description can be found.

Process Architecture In the last decades, a major part of the existing processes has been optimised substantially, among other things by using more advanced process control and by using pinch and exergy analyses. The gain that can be reached in this way, however, has gradually decreased. In order to reach breakthroughs, it is essential to develop new process concepts, which can lead to inherently 'green' processes. In general, a radical innovation is acceptable to the market if it gives a 5 to 10-fold improvement at half the costs.
The theme of Process Architecture comprises two related sub-themes, *viz.* Chemistry Intensification and Novel Process Routes. See for more details Annex 1.

Process Intensification Process Intensification (PI) aiming at 'Smaller and Smarter, Cheaper and Safer' is part of the answer of GSPT to the need for flexibility in production and compact installations and to pressure from society towards more sustainable production processes. Within the framework of the development of sustainable process technology, PI is the counterpart of 'changing the process chemistry' as PI is concerned with process development and usually focuses on plant and equipment design. PI re-considers the principles of design and looks for new technology that can achieve a 1/3 or more improvement in the cost of investment and operation, floor use of the site, use of energy and raw materials, and/or waste streams. See for more details Annex 1.

Enabling Technologies Modelling and computational simulations may really contribute to GSPT. The use of computational tools eliminates the traditional approach of step-wise scale up involving pilot plants. In addition, we need to focus on scale down as well. For both, computational chemical engineering – linking the molecular, the mesoscopic and the macroscopic scales – is of vital importance. This is a theme that shows up in many of the roadmap documents produced in the USA in recent years: *e.g.,* a focus on R&D in the field of Computational Fluid Dynamics (CFD) was identified in '*Technology Vision 2020*: *The US Chemical Industry'* (ACS *et al*., 1996) as a high-priority issue for meeting industry's future goals. See for more details Annex 1.

4.3. Important remarks on GSPT-programme

Finally, it is emphasized that in GSPT the leading role has been reserved for process technology, with additional contributions from fields such as industrial catalysis, chemistry, thermodynamics, materials science, micro-system technology, transport phenomena, computational technologies, and process control. The idea is to build on existing knowledge and expertise in the various sub-fields and to combine these in a multidisciplinary effort towards an integrated solution, either in terms of a novel process route or architecture, or of a new reactor configuration or process intensification mode, anyhow with the view to make a big step forward in sustainability, economy, safety, *et cetera*. Basic studies in the above fields *per se* do not qualify for support within GSPT. Demonstrating the viability of a process or reactor concept could well be part of a research proposal.

5. Het STW-programma

5.1. Onderscheidende karakter van het programma

In de hoofdstukken 1 t/m 3 zijn de algemene kaders van dit GSPT-onderzoeksprogramma geschetst. Met name is het onderzoekskader weergegeven in sectie 3.2 en in Annex 1, waarbij de gekozen thema's en onderwerpen in meer detail zijn beschreven. Hieruit blijkt dat dit GSPT-programma een herkenbaar technologieprogramma is, met een basis in de procestechnologie. Het programma richt zich op de ontwikkeling van (delen van) nieuwe en innovatieve reactoren, procesapparatuur en processystemen voor de productie van bestaande en nieuwe chemicaliën. Belangrijke aandachtspunten zijn verbetering en optimalisatie van producteigenschappen, selectiviteiten en opbrengsten, en het ontwikkelen en exploreren van nieuwe of alternatieve chemische syntheseroutes. Doel van het GSPT-programma is deze schone ("Green") chemie mogelijk te maken met behulp van innovatieve en slimme ("Smart") processen.

Het succes van het programma wordt gevormd door de mate waarin een vruchtbare samenwerking gerealiseerd zal worden tussen verschillende wetenschappelijke en technologische disciplines. De doorbraken in technologievernieuwing worden daarbij verwacht op de raakvlakken van disciplines als fysica, chemie, biologie, fysische chemie, colloïdchemie, industriële katalyse, materiaalkunde, chemische technologie, procestechnologie, fysische technologie, regeltechniek, en ook microfabricagetechnologie. Deze multidisciplinaire aanpak onderscheidt dit GSPT-programma van andere onderzoekprogramma's die zich voornamelijk richten op één vakgebied, discipline, of technologie.

Het GSPT-programma onderscheidt zich derhalve van thans lopende nationale en internationale onderzoeksprogramma's die op enigerlei wijze raakvlakken hebben of verwant zijn aan het GSPT-programma, zoals Process on a Chip (PoaC), MicroNed, ASPECT, DSTI, IBOS, B-BASIC, en IMPULSE. Het GSPT-programma heeft dus een duidelijk eigen en uniek profiel. Binnen het Open Technologieprogramma van STW zijn reeds een aantal projecten binnen dit onderzoeksveld gestart.

Het PoaC-programma van NWO-ACTS [12] richt zich voornamelijk op de ontwikkeling van nieuwe chemische producten en syntheseroutes voor specifiek de fijnchemische en farmaceutische industrie. De productiecapaciteit en gerelateerde apparatuur zijn zeer kleinschalig, met name gerelateerd aan (silicium)chipgebaseerde toepassingen. Belangrijke aspecten zijn tevens *in situ* metingen van producteigenschappen en procescondities.

MicroNed [13] richt zich voornamelijk op ontwikkeling van nieuwe fabricagetechnologie voor microsystemen voor uiteenlopende toepassingen. Een klein onderdeel in het MicroNed-programma richt zich op ontwikkeling van microreactoren, met een sterke focus op de fabricagetechnologie in samenwerking met gespecialiseerde microtechnologie-georiënteerde bedrijven.

Het ASPECT-programma van NWO-ACTS [14] biedt slechts in beperkte mate de mogelijkheid om projecten in te dienen gericht op microreactortechnologische toepassingen bij bulkchemische productie.

Het recent opgerichte DSTI (Dutch Separation Technology Institute) [15] richt zich op de ontwikkeling en demonstratie van nieuwe scheidingstechnologieën. Een toekomstige samenwerking met DSTI ligt voor de hand gegeven de uitdagende mogelijkheden en voordelen van integratie van reactie en scheiding.

Het IBOS-programma van NWO-ACTS [14] richt zich op integratie van biosynthese en organische synthese middels combinatie van moderne biochemische concepten en biotechnologie.

Het B-BASIC-programma van NWO-ACTS [14,16] richt zich op de ontwikkeling van nieuwe biogebaseerde productieconcepten voor de chemische en de energie-gerelateerde industrie. Het programma baseert zich op nieuwe inzichten in de moleculaire biologie (o.a. genomics) in combinatie met geavanceerde bioprocestechnologie. Er worden ondermeer processen ontwikkeld voor omzetting van biomassa in chemische producten met behulp van nieuwe biokatalysatoren zoals microorganismen en enzymen.

Het Europese IMPULSE-project (in het zesde Kaderprogramma van de EU) [17] richt zich op integratie van innovatieve procesapparatuur (m.n. micro- en mesogestructureerde reactoren, mengers, scheiders, warmtewisselaars, enz.) in complete processystemen voor chemische en farmaceutische productie. Het project beoogt procesintensificatie te bereiken door optimalisatie van het ontwerp van procesapparatuur op verschillende lengteschalen. Er is geen deelname van Nederlandse bedrijven of universiteiten.

Verder zijn er recente initiatieven bekend voor het realiseren van samenwerkingsverbanden en gerelateerde onderzoeksprogramma's die verwantschap hebben met het GSPT-programma, zoals het Procesintensificatie Netwerk Nederland (PIN NL) [18]. Hiermee zijn goede kontakten, die in de toekomst kunnen leiden tot verdere afstemming, samenwerking en differentiatie.

Dit programma is tot stand gekomen na een voortraject waarbij eerst in klein comité een inventarisatie is gemaakt van 'het speelveld', zie 'drivers and research themes' in Annex 1. Hierbij waren de heren Van den Akker (TUD), Alderliesten (ECN), Bargeman (Akzo), Kwant (DSM) en Marcelis (STW) betrokken. De reden om deze inventarisatie op te starten is de invulling van de nieuwe programmatische aanpak van STW.
De resultaten van de inventarisatie zijn voorgelegd in een workshop met bedrijven, universiteiten en kennisinstellingen. In de workshop is het draagvlak voor en de focus van het programma voor de achterban getoetst. Dit heeft geleid tot deze programmabeschrijving met bijdragen van: Van den Akker (TUD), Alderliesten (ECN), Bargeman (Akzo), Kwant (DSM), Stankiewicz (TUD/DSM) en Schouten (TU/e).

[12.] http://www.nwo.nl/nwohome.nsf/pages/NWOA_6NSHCF_Eng
[13.] http://www.microned.nl/
[14.] http://www.nwo.nl/nwohome.nsf/pages/NWOP_5SKDNM?opendocument&nav=ASPECT_02_Eng
[15.] http://www.scheidingstechnologie.nl/publicdocs/pressreleaseDSTI.doc
[16.] http://www.b-basic.nl/index.html
[17.] http://www.impulse-project.net/
[18.] http://www.technology.novem.org/en/process-intensification/start.htm

5.2. Organisatie van het programma

5.2.1. Procedure

Voor dit programma is een bedrag van M€ 5.5 beschikbaar, waarvan minimaal 25% moet worden bijgedragen door potentiële technologiegebruikers (bedrijven en/of kennisinstellingen). De participanten kunnen dus per project bijdragen en hoeven geen upfront cofinanciering voor het hele programma te leveren.

Aanvragen kunnen worden ingediend door medewerkers van Nederlandse instellingen voor Wetenschappelijk Onderwijs en de door NWO erkende instituten. Omdat het GSPT-programma expliciet multidisciplinair is opgezet moeten minimaal twee verschillende onderzoeksgroepen bij een project betrokken zijn. Uit het voorstel moet de multidisciplinaire aanpak duidelijk blijken.

Naast een bondige beschrijving van de te verwachte resultaten en de onderzoeksplanning moet een utilisatieparagraaf worden geschreven. In de utilisatieparagraaf moet duidelijk worden gemaakt welke voor de industrie relevante probleemstelling wordt opgelost en op welke termijn implementatie van kennis in de praktijk verwacht kan worden. Potentiële gebruikers van kennis moeten bottom-up bij de projecten zijn betrokken. Pre-proposals moeten worden voorzien van intentieverklaringen van de participanten In deze verklaring geven zij aan dat zij kennis hebben genomen van de utilisatieparagraaf en deze onderschrijven. Verder moet uit de verklaring duidelijk worden dat de potentiële gebruiker in principe bereid is om bij te dragen aan het project.

De pre-proposals zullen door een programmacommissie worden gerangschikt op basis van hun inpasbaarheid in het programma, de wetenschappelijke kwaliteit (in termen van originaliteit, innovatief karakter en haalbaarheid) en het toepassingspotentieel. Voorafgaand aan een plenaire bespreking van de pre-proposals zullen de leden van de programmacommissie onafhankelijk van elkaar de voorstellen op deze drie criteria scoren. Bij de plenaire bespreking wordt ook de focus van het totale programma meegenomen in de discussie. Op basis van het oordeel van de programmacommissie ontvangen de indieners een positief of negatief advies om het pre-proposal uit te werken tot een volledige aanvraag.

De uitgewerkte voorstellen worden na een internationale referentenronde (‘peer review’) met hoor en wederhoor geprioriteerd door een onafhankelijke deskundige jury op basis van wetenschappelijke kwaliteit en het utilisatiepotentieel. De jury zal bestaan uit vertegenwoordigers van Nederlandse bedrijven en kennisinstellingen en buitenlandse academici. De programmacommissie stelt aan de hand hiervan een honoreringsvoorstel op, het bestuur van STW zal besluiten welke voorstellen worden gehonoreerd.

Bij de uitgewerkte voorstellen is een definitief commitment van de participerende bedrijven en/of kennisinstelling verplicht, zodat duidelijk uit het budget blijkt hoe de minimale bijdrage van 25% van de totale projectkosten is opgebouwd. Dit moet worden vastgelegd in een ‘letter of participation’.

Bij de beoordeling van de aanvragen spelen de volgende selectiecriteria een rol:

Wetenschappelijke kwaliteit:
- Originaliteit en innovatief karakter van het onderzoeksvoorstel
- Verwachte impact en bijdrage van het onderzoek aan de wetenschappelijke kennis
- Onderzoeksmethode, haalbaarheid, tijdfasering en beschikbare infrastructuur
- Coherentie, afstemming en synergie
- Budget
- Reputatie, samenstelling en ‘past performance’ van de aanvragers

Utilisatie:
- Bijdrage aan de ontwikkeling van toepasbare kennis van belang voor potentiële gebruikers.
- Bruikbaarheid van resultaten op langere termijn voor een (commerciële) toepassing.
- Mogelijkheid tot de ontwikkeling van beschermwaardige kennis (octrooiering).
- Participatie van (commerciële) gebruikers en identificatie van alternatieve gebruikers.

5.2.2. Budget

De maximale omvang van een project is 1 miljoen euro. In het kader van een onderzoeksproject kan het volgende worden aangevraagd:

- AIO posities
- Postdoc posities (36 maanden maximaal)
- Posities voor tijdelijk technisch personeel (36 maanden maximaal)
- Budget voor verbruiksgoederen
- Apparatuur
- Reiskosten voor tijdelijk verblijf elders van onderzoekers om zich specialistische kennis en/of vaardigheden eigen te maken of voor congres/workshopbezoek.

Cofinanciering van gebruikers kan in geld of in-natura. Voor in-natura bijdragen gelden de volgende randvoorwaarden:

a) Apparatuur kan worden ingebracht als deze wordt opgevoerd tegen de kostprijs en rekening wordt gehouden met reeds gedane afschrijvingen.

b) Het is mogelijk dat een gedeelte van het onderzoek wordt uitgevoerd door derden (industriële partner of kennisinstelling). Een bijdrage in mensuren moet voldoen aan de volgende criteria:

- Het gedeelte dat door een gebruiker wordt ingebracht moet integraal onderdeel uitmaken van het totale werkplan. De subject matter experts van de betreffende bedrijven/instellingen participeren actief bij de bijeenkomsten van de gebruikercommissie.
- Voor het berekenen van de bijdrage door derden (minimaal 25%) bij de behandeling van het project wordt uitgegaan van een uurtarief van 106 €. Dit tarief is gebaseerd op de loonkosten van een senior onderzoeker vermeerderd met een opslag van 100%.
  In de brieven van bedrijven ter ondersteuning van de full-proposals moeten het aantal uren worden benoemd. Het aantal uren moet corresponderen met de milestoneplanning in het voorstel.
  Gezien het internationale karakter van de beoordelingsprocedure moeten brieven ter ondersteuning van het voorstel in het Engels worden gesteld.

Voor overige details wordt verwezen naar de richtlijnen voor het open technologieprogramma (www.stw.nl).

5.2.3. Platformfunctie

De voortgangsbewaking, het financieel en administratief beheer wordt uitgevoerd door STW. STW zal ook de programmacommissie faciliteren. We willen een hechte en blijvende samenwerking realiseren tussen academie, instituten en bedrijfsleven (waaronder ook het MKB!). Hier ligt ook een rol voor de programmacommissie, die de samenhang van het programma bewaakt en de kennisuitwisseling tussen academie en partners en overdracht van IP (intellectual property) naar de partners stimuleert.
Daarnaast zal de programmacommissie een rol spelen in het tot stand komen van een strategische onderzoeksagenda rond de toepassing van schone chemie in innovatieve slimme productiesystemen door het oprichten van een platform of aansluiting te zoeken bij bestaande platform-initiatieven.

5.2.4. Valorisatie

Per project wordt een gebruikerscommissie ingesteld waarin naast de inhoudelijke voortgang aandacht wordt besteed aan het benutten van kansen om technologie over te dragen naar gebruikers. Met betrekking tot IP & licencing wordt het reguliere beleid van STW gevolgd. STW streeft er naar om octrooien aan te vragen indien er een duidelijk financieel commitment van potentiële gebruikers is om bij te dragen in de kosten van het octrooi en de kennisbescherming en exploitatie verder gezamenlijk aan te pakken.

5.3. Indiening voorstellen en tijdpad

De deadline voor de indiening van pre-proposals is 12 januari 2007. Het tijdschema van de beoordelingsprocedure is als volgt (wijzingen voorbehouden):

Call for pre-proposals	26 oktober 2006
Sluitingsdatum indiening pre-proposals	12 januari 2007
Beoordeling door programmacommissie	19 januari 2007
Sluitingsdatum indiening full-proposals	2 maart 2007
Beoordeling door referenten inclusief wederhoor	6 april 2007
Prioritering jury	20 april 2007
Honoreringsbesluit	eind april 2007

Annex 1

6. Annex

A detailed description of the GSPT programme for potential applicants

1. A more detailed description of the themes eligible within GSPT

GSPT encompasses novel process architectures and process intensification, and is facilitated by recent advances in computer technology, simulation capabilities and process synthesis. These themes are discussed below in more detail.

Process Architecture In the last decades, a major part of the existing processes has been optimised substantially, among other things by using more advanced process control and by using pinch and exergy analyses. The gain that can be reached in this way, however, has gradually decreased. In order to reach breakthroughs, it is essential to develop new process concepts, which can lead to inherently 'green' processes. In general, a radical innovation is acceptable to the market if it gives a 5 to 10-fold improvement at half the costs.
The theme of Process Architecture comprises two related sub-themes, *viz.* Chemistry Intensification and Novel Process Routes.

Chemistry Intensification As the current chemical industry relies on a chain of plants each optimised for a single chemical reaction, it is obvious that a major improvement of process economics and environmental load could be obtained by combining consecutive steps in a single plant provided that an acceptable efficiency can be reached. This concept is denoted by the term 'Chemistry Intensification'. It particularly bears to fine chemicals and pharmaceuticals.

Chemistry intensification means shortening chemical pathways, by combining or integrating reaction steps or by using different, more active or more selective catalysts (without implying that extensive catalyst screening and testing could be part of the research proposal). The use of direct addition reactions should be explored rather than the detour via substitution reactions. Concepts such as atom efficiency should be exploited to a higher degree as well. Maintaining product properties during scale up is also an issue, in particular when the round bottom flasks used by the chemists have to be replaced by full-scale process equipment of a different kind.

Chemistry intensification aims at stimulating the development of concepts which enable to shorten the chain of chemical plants necessary for the production of the final product either by performing reactions in cascade in a single reactor or by using intermediates which are produced by integrated reaction sequences. It is really about 'changing the process chemistry'.

Chemistry intensification may result in tremendous decreases of energy consumption and waste production as well as in an improvement of plant economics (in numerous of these intermediate steps, more waste is produced than final product).

Novel process routes Chemical industry strongly relies on feedstocks and processes developed decades ago. In that time, environmental issues were less important than nowadays; as a result, these issues did not play an important role in process economics. Since those days, however, environmental awareness has increased tremendously. So far, this did not result in many replacements of established processes by novel, greener routes. Many processes still make use of organic solvents and of heterogeneous catalysts of inferior selectivity. New chemical routes might be considered, by revisiting the position of any process in the nowadays-worldwide network of companies and plants.

In addition, it is evident that - in view of the envisaged future feedstocks - novel routes are to be implemented in bio-feed or biochemical processes. As future feedstocks may often be oxygenated compounds and hydrogen is probably the fuel of tomorrow, it can be anticipated that selective hydrogenation will gain in importance. It would be a challenge to design and exploit heterogeneous reduction catalysts with a high resistance against poisoning with CO. Bio-based processes might lead to the use of a number of bulk chemicals as monomers, *e.g*. lactic acid, citric acid, acetone, butanol, ethanol, acetic acid, aspartate, malate, lysine, and even caprolactam._These developments may stimulate the development of entirely new alternative pathways to the products of the bulk chemical industry.

Process Intensification (PI) aiming at 'Smaller and Smarter, Cheaper and Safer' is part of the answer of GSPT to the need for flexibility in production and compact installations and to pressure from society towards more sustainable production processes. Within the framework of the development of sustainable process technology, PI is the counterpart of 'changing the process chemistry' as PI is concerned with process development and usually focuses on plant and equipment design. PI re-considers the principles of design and looks for new technology that can achieve a 1/3 or more improvement in the cost of investment and operation, floor use of the site, use of energy and raw materials, and/or waste streams.

These tough targets may be met by, among other things, introducing new reactor types among which multi-functional reactors, structured reactors (*e.g.*, catalytic monolith systems) or micro-reactors, or by introducing more profitable conditions such as cyclic or transient operation, or 'exotic' aids such as electric fields, enhanced gravity or strongly swirling motions.

PI is also about combining functions into a single piece of equipment, preferably at a smaller size, too. PI goes beyond the familiar approach of connecting unit operations in series, each unit operation being carried out in a separate piece of equipment. PI avoids thinking in terms of equipment; it rather emphasizes the functions to be effected and looks for ways to realize them in a form as compact as possible.

Many (fine) chemical processes are operated batch-wise. Stirred batch reactors are assumed to be flexible and are therefore commonly used, but in practise they suffer from significant disadvantages. Switching to continuous processing has been applied in various industrial cases resulting in significant improvements.

In recent years, quite some attention is being paid to the promises of carrying out processes in micro reactors. Doing this may exhibit distinct advantages when compared to traditional production procedures.

Enabling technologies Modelling and computational simulations may really contribute to GPT. The use of computational tools eliminates the traditional approach of step-wise scale up involving pilot plants. In addition, we need to focus on scale down as well. For both, computational chemical engineering – linking the molecular, the mesoscopic and the macroscopic scales – is of vital importance. This is a theme that shows up in many of the roadmap documents produced in the USA in recent years: *e.g.,* a focus on R&D in the field of Computational Fluid Dynamics (CFD) was identified in *Technology Vision 2020* as a high-priority for meeting the industry's future goals.

Exploiting computational simulations will improve performance in two ways: (a) the amount of resources spent and waste produced during scale-up will be minimised by reducing the number of testing stages, and (b) the improved process synthesis/design methods will produce more efficient processes. In addition, computational technologies may assist in identifying potentially novel process routes and reactors (operating conditions, reactor geometries, safety margins). Advanced CFD should capture and mimic the complexity of real systems at fine scales; this may be particularly important for multiphase systems that currently are still extremely difficult to scale up.

By incorporating detailed chemistry, reaction kinetics and transport processes, the models will determine selectivity and even predict production of by-products at trace levels in side reactions. Integrated modelling of reactions and downstream processing will provide complete reaction and reactor synthesis tools suitable for systems-level assessment of safety and economics.

The models of the future cannot be developed without experimental input and verification. New ideas for lab reactors are needed to improve the efficient collection of complete and accurate kinetic data. Better characterisation of lab-scale and full-scale reactors is needed, coupled with a better understanding of the effects of transport phenomena on reaction processes by computational simulation at various time and length scales.

The novel processing concepts developed in the above two themes Process Architecture and Process Intensification also need to be translated into conceptual process designs that can be flexibly operated in a sustainable way. These designs must also consider the operational features of a process, *i.e.* dynamics, controllability, reliability and availability.

In addition, the fast pace of developments in modelling and computing technology will present a new range of options for improved design and optimisation tools, capable of dealing with larger numbers of first-principles equations in models and of handling much larger “inverse problems” (*i.e.*, finding those process structures that exhibit pre-specified behavioural features).

2. Drivers and research themes

In the Table below, we summarise a number of drivers for a concerted GSPT effort. We further identify a non-exhausting list of issues and related research topics and sub-disciplines that could contribute to the multidisciplinary GSPT programme. We repeat once more that process technology should take the lead, that the emphasis should be on process and/or reactor, and that the development of science or of enabling technologies will only be allowed as far as they contribute to the purpose of the ultimate goals as described in *e.g.* the Ambition in Chapter 1 of this document.

Driver: product quality

Issues	Possible Research Topics (not exhaustive, just to guide thinking)
Properties, specifications, purity	Control: sensors on line and in-situ Control of hydrodynamics (Micro) structured reactors and catalysis engineering

Driver: costs

Issues	Possible Research Topics (not exhaustive, just to guide thinking)
Selectivity and yield	(Micro) structured reactors Integration / in-situ product recovery Mixing control
Alternative chemical routes	Atom efficiency and catalysis engineering Molecular modelling (Micro) structured reactors
Heat recovery	Modelling and model predictive control Intensified equipment
Degree of automation	Process modelling and simulation Process analytics
Low investments	Computational simulations (making pilot plants and scale-up issues redundant) Intensified equipment Numbering up and scale out

Driver: Legislation and licence to operate in the Netherlands

Issues	Possible Research Topics (not exhaustive, just to guide thinking)
Safety	Batch to continuous processes (Micro) structured reactors Alternative reaction paths
Green resources	Feed stock preparation Alternative reaction paths
Emission reduction	Closed loop (chain) Solvent free processing

Driver: Functionality

Issues	Possible Research Topics (not exhaustive, just to guide thinking)
New / improved product properties	Control and definition of specifications Control of mixing/emulsions Physical properties defined in reactors under operational conditions
(Continuous) multi-purpose reactors	Application of simulation technology Down-sized production systems Modular systems
High capacity (heat removal, mixing)	(Micro) structured multiphase systems
On site production for customer	(Micro) structured reactors Extreme conditions

Driver: Energy

Issues	Possible Research Topics (not exhaustive, just to guide thinking)
Heat loss reduction	Heat recovery Catalysis engineering Molecular modelling
Low energy routes, integration	Reaction modelling Process synthesis
Upgrade of energy for re-use	Waste based processes
Alternative transfer processes	Light-, ultrasound-, microwave-, plasma-based processes

Peer Group

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Wednesday, 06 December 2006