

Technology Roadmap Catalysis

Catalysis, KEY TO SUSTAINABILITY

DRAFT Final Report
Technology Roadmap Catalysis
June 2001

Acknowledgements

In the Technology Roadmap Catalysis process an R&D-plan for the next 10 years for catalysis in The Netherlands has been developed by the catalysis field itself. This report provides an overview of the results.

Due to the diverse nature of catalysis in technological terms (e.g. homogeneous, heterogeneous, and bio-catalysis, process and reactor technology, etc.) and the broad range of organisations involved in catalysis R&D (commercial industries, research organisations, universities and governmental bodies) this project required assistance from many sources. Many organisations and individuals contributed to the final result through their input in personal interviews, three TRM-workshops with approximately 50 persons per workshop, a final work-conference with approximately 100 participants. Many others have provided valuable insights and information on the sideline.

When help is received from so many sources (a list of contributors to the process can be found in the Annex), it is impossible to individually thank everyone who contributed to the final results. We thank all of them.

Some people however played an essential role in the Technology Roadmap Catalysis process. These are the members of the TRM Catalysis Core Team and Sounding Board.

The TRM Catalysis Core Team

The members of TRM Catalysis Core Team represented the broad field of catalysis in The Netherlands with participation of industrial organisations and the knowledge infrastructure. The Core Team served as a platform providing content for the workshops (in the form of discussion documents) and subsequently writing the main part of this Technology Roadmap Catalysis report. Besides their strong efforts and substantial investments in time to write the discussion documents and final report, they participated in the workshops and in multiple core team meetings. Without the personal investments of each of the individual core team members this roadmap could not have been created.

The Core Team of the Technology Roadmap Catalysis consisted of, in alphabetical order:

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The Sounding Board

The members of the Sounding Board provided guidance on the scope and approach of the roadmapping process. In regular meetings they provided us with suggestions and feedback on the plans, progress and (interim) results enabling us to further streamline the process in order to maximise the results.

The Sounding Board for the Technology Roadmap Catalysis consisted of, in alphabetical order:

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- Dr. F. van den Brink, *DSM / VIRAN*
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1. INTRODUCTION

This introduction is meant to serve as a guide in reading this Technology Roadmap Catalysis (TRM-Catalysis) document and will subsequently cover:

- Background, goal and scope of the TRM-Catalysis
- The roadmap methodology and approach
- Guide to the TRM-Catalysis graphs and technology tables

Background, goal and scope of the TRM-Catalysis

In the summer of 2000 the Dutch Ministry of Economic Affairs took the initiative for the development of a technology roadmap catalysis project. This roadmapping process aimed at the development of a vision on the future of catalysis, setting clear goals for catalysis research and development projects, improvement of co-operation and joint research and development within The Netherlands. The TRM-Catalysis should provide a framework for joint industry and university R&D programmes, thus strengthening the overall Dutch catalysis network and its international position.

PricewaterhouseCoopers N.V. has been the facilitator of the technology roadmap process.

Background

The technology roadmap was initiated as a result of the Technology Radar; a technology forecast study of PricewaterhouseCoopers N.V., published in 1998. In this study catalysis was earmarked as a strategic technology within The Netherlands. A subsequent Radar workshop with a focus on catalysis with representatives from industry, research organisations and relevant governmental bodies was held in May 1999 in order to discuss the future of catalysis in The Netherlands.

The main conclusions from the Technology Radar and the Catalysis workshop were:

Catalysis is of major importance for the Dutch economy

The chemical industry generates 20-30% of the Dutch gross national product. The total turnover in the Netherlands of catalysis related activities tops 50 billion Dutch guilders. About 80% of all chemical processes used for the production of a wide variety of chemical products use catalysis. Knowledge of catalysis is not only of major importance for the economics of these processes, but also for the development of environmental and energy friendly processes. Catalysis is therefore seen as a key factor within the Dutch (chemical) industry. From this perspective it is clear that catalysis is of strategic importance.

Catalysis knowledge and R&D capability within The Netherlands also proved to be internationally strong and broad in scope. Its national organisational structures are well developed and they benefit from the fact that they are geographically close to each other. Furthermore, communication within the field of catalysis is frequent and open, using platforms such as the IOP-Katalyse programme. Researchers from the industry, universities and other knowledge institutes often know each other and their respective capabilities related to the field.

Identified strategic challenges in Dutch catalysis need to be addressed

However, not all was judged positive. The following strategic issues were identified as challenges for the Dutch Catalysis network:

- a. Threat of a widening R&D gap:** A widening gap was perceived between fundamental, university based, long-term research and short-term industrial applied research and development. Recent years showed a reduction in industrial R&D budgets, the nearing end of governmental funding of NIOK and the IOP-Catalysis research programme and a shift to more fundamental research at universities. These developments cause a widening gap between the medium term and the strategic R&D, which needs to be addressed.
- b. Diminishing interaction:** Communication in the field of Catalysis depends partly on the availability of platforms such as IOP-katalyse, NIOK (the Dutch research school which combines multiple universities) and its industrial counselling Board VIRAN, GBB and OSPT. With the end of the IOP-programme and the retreat of the Dutch government in terms of financial backing for NIOK and VIRAN, communication may be affected. This, combined with the widening R&D gap, may cause the interaction between industry and the knowledge infrastructure to diminish. Specifically the selection and definition of research topics as well as joint funding and execution of research programmes are issues in need of attention.
- c. Lack of qualified researchers:** The Netherlands has, and still experiences, a significant drop in the number of students and post-docs at universities in science and technology disciplines. The catalysis related disciplines are also affected. This causes problems in fulfilling research and development related vacancies in industry, universities and other research organisations. This issue requires a solution in order to maintain and further develop the science and technology base in The Netherlands in terms of international competitiveness.

Need for joint strategic catalysis R&D programme

The Radar-Workshop participants agreed on the need to fill the R&D gap with a strategic R&D programme in which long-term priorities are set for economic application of catalysis. Such a programme needed to be more than a collection of loose and ad-hoc financed projects. It should provide a coherent framework based on a number of prioritised themes. The selected way ahead was to continue and intensify the dialogue between industry, knowledge infrastructure and governmental bodies based on a technology roadmapping approach. The technology roadmap exercise would serve as a tool and platform to set priorities, define a coherent R&D programme and build the catalysis network.

TRM catalysis goals

Based on the issues as described above the Ministry of Economic Affairs has taken the initiative for the development of a technology roadmap catalysis and asked PricewaterhouseCoopers N.V. to facilitate the process.

The main reasons to initiate this roadmap are:

- a. To prepare for ambitious demands in the next 10 to 20 years:** The impact of catalysis and its related technologies on the economics and sustainability of products and processes in a large range of industry sectors is substantial. Developments however are rapid and the international playing field necessitates a continued investment and effort to stay “best of class” in catalysis. In order to do so it is necessary to identify the main challenges for catalysis in the next 10 to 20 years and prepare for them by initiating collaboration and R&D projects aligned with these challenges.
- b. To enhance research collaboration between industry and universities:** The widening gap between short term applied R&D and long term fundamental R&D is strongly related to the differences between the industrial and university views on the goals of and approach to R&D. The potential gains which can be achieved through synergy when both R&D types are combined are large. Enhanced collaboration between industry and universities within catalysis will enable both sides to benefit.
- c. To strengthen the "Catalysis" network through concrete actions and projects:** The catalysis network in The Netherlands provides the basis for communication, collaboration and a strong international position. Concrete actions and projects based on joint needs and priorities will further strengthen this network and provide a backbone for the continued and improved strong international position of Dutch catalysis.

TRM catalysis scope

The scope of the TRM Catalysis is defined by the fact that the Technology Roadmap Catalysis will serve as an **ambitious** and **long-term** joint R&D plan for the organisations active within the field of **catalysis** in **The Netherlands**. From the start, the roadmapping initiative has been set up as an effort of the organisations active within the catalysis field itself. Input and choices of the core team, workshop participants and the Sounding Board have shaped the roadmap and the priorities set in it.

This approach in the development of the TRM Catalysis meant that the scope was determined by:

Ambitious: Focus on major technological challenges within catalysis

The Technology Roadmap Catalysis is not intended to provide a full and utterly complete and detailed overview of all possible catalysis related R&D challenges and programmes. It has been decided from the start that the efforts would be focussed at identifying areas in which catalysis will play a key role and at technological breakthroughs. The related development routes should be detailed to a level on which the involved organisations could base joint proposals for R&D programmes and/or projects.

This has resulted in:

- a. Use of high-priority goals:** During the workshops with the TRM core team and the catalysis field the main challenges for catalysis have been defined in the form of “high-priority goals”. These high-priority goals, signifying key business and societal needs, have served as basis for the subsequent identification and detailing of the development routes ensuring a focus on key challenges for catalysis in the roadmap.
- b. Use of challenging goals:** The high-priority goals have been specified, where possible, in (quantitative) targets. These targets have been set in order to provide a tangible challenge for catalytic R&D efforts. These goals and quantified targets have been, and should be, used for TRM purpose only. Use and/or communication of these targets should only be done with clear reference to the TRM Catalysis project and its context.
- c. Technology as main focus:** The Catalysis roadmap has focussed mainly on technological issues and to a significantly lesser extent on commercial and financial feasibility. They are however of paramount importance in the choices for and execution of R&D projects as well as the implementation of the resulting technologies and they must always be taken into account.

A forecast and planning of technological R&D in the field of catalysis must always leave room for unexpected developments, inventions and breakthroughs. This roadmap has not explicitly included such events in the report as they are not predictable but acknowledges the potential impact of unexpected technological breakthroughs. A consequence is that this Technology Roadmap Catalysis is not a static document and periodic re-evaluation of its contents is needed.

Long-term: Focus on 10 year-period

In the TRM Catalysis a period of 10 years has been used in defining the business and societal needs which could be (partly) fulfilled by catalysis. This period was chosen in order to capture challenging future demands and breakthrough developments while assuring a strong link to real implementation and integration with current R&D efforts.

Catalysis: Broad technological and organisational perspective

In The Netherlands a broad range of activities exists in the field of catalysis. The roadmap aims to capture the variety in three areas:

- a. Technologies:** Catalysis is a broad technological field which includes a wide variety of technologies. In this TRM-Catalysis the participants have defined the scope of technologies to be included. Main considerations are:
 - In the discussions and in this report Catalysis has been defined as the combined fields of heterogeneous, homogeneous and bio catalysis;
 - Catalysis is also closely related to other technological fields of research and development, the scope of the technology roadmap project includes areas such as reactor design, separation technologies, material science, organic chemistry, physics, etc.

- b. Organisational:** The project has involved a broad range of organisations active in the field of catalysis within The Netherlands. No limitations have been placed on participation of individual organisations from the start.
- **Industry sectors:** In terms of industrial sectors the Technology Roadmap Catalysis focused on the chemical and related industries in a broad sense. The only restrictions in industry sectors resulted from the representation of the industrial companies in the process (some sectors were actively stimulated to contribute to the process) and choices made by them during the workshops.
 - **Knowledge infrastructure:** The project included the full range of Dutch catalysis research. Besides the industrial research and development, the Technology Roadmap Catalysis received input from university research groups, as represented by NIOK (University of Amsterdam, Delft University of Technology, Eindhoven University of Technology, Groningen University, Leiden University, Twente University of Technology, Utrecht university and Wageningen Agricultural University), OSPT and GBB and other research organisations (such as ECN and TNO).
 - **Government:** The TRM-Catalysis was initiated as a development effort of the catalysis field itself, consisting of industrial and research organisations. The government (Ministry of Economic Affairs) initiated the process but did not actively steer in the content or priorities set by the catalysis field.

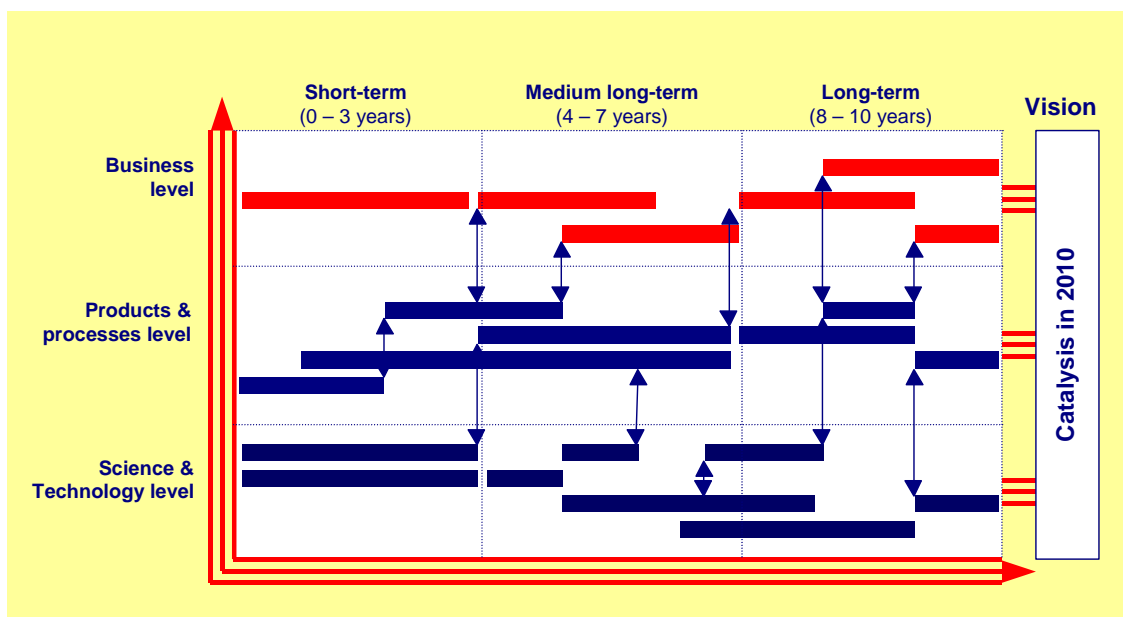
The Netherlands: Focus on The Netherlands but with international perspective

The main focus in the TRM-Catalysis has been organisations active within The Netherlands. This however does not imply that the strong international context of technological developments related to catalysis has been ignored. On the contrary; based on a broad, in-depth and international understanding of catalysis and its expected future developments, the implications for the Dutch catalysis network have been identified and reflected in the choices and priorities in the roadmap. The international perspective is also reflected by the fact that the participating organisations all (both industrial and universities) have international working areas and contributed to the TRM-Catalysis based on their international knowledge in the field.

The TRM-Catalysis methodology and approach

Methodology

The approach used a needs-driven technology planning process that helps to identify, select and develop technological alternatives which fulfil a set of future needs. The roadmapping approach assists in identification, matching and planning of research and development efforts in specific market, product/process, technology combinations (MPTCs). The main consideration was to link the societal and industrial future needs to catalysis science and technology.



Picture 0.1: Technology Roadmap Methodology

Characteristic elements in the TRM methodology are:

- a. **Vertical segmentation:** reflecting the business, product/process and technology combinations (MPTC's) consisting of:
 - **Business level:** Defined by high-priority goals reflecting the societal and industrial needs over time;
 - **Product / process level:** Defined by the products and/or processes which have an impact on the established high-priority goals which will be the basis for the development routes;
 - **Technology level:** Defined by the technologies/sciences needed in the R&D efforts.
- b. **Horizontal segmentation:** reflecting the time zones:
 - Short-term: 0 to 3 years
 - Medium long-term: 4 to 7 years
 - Long-term: 8 to 10 years

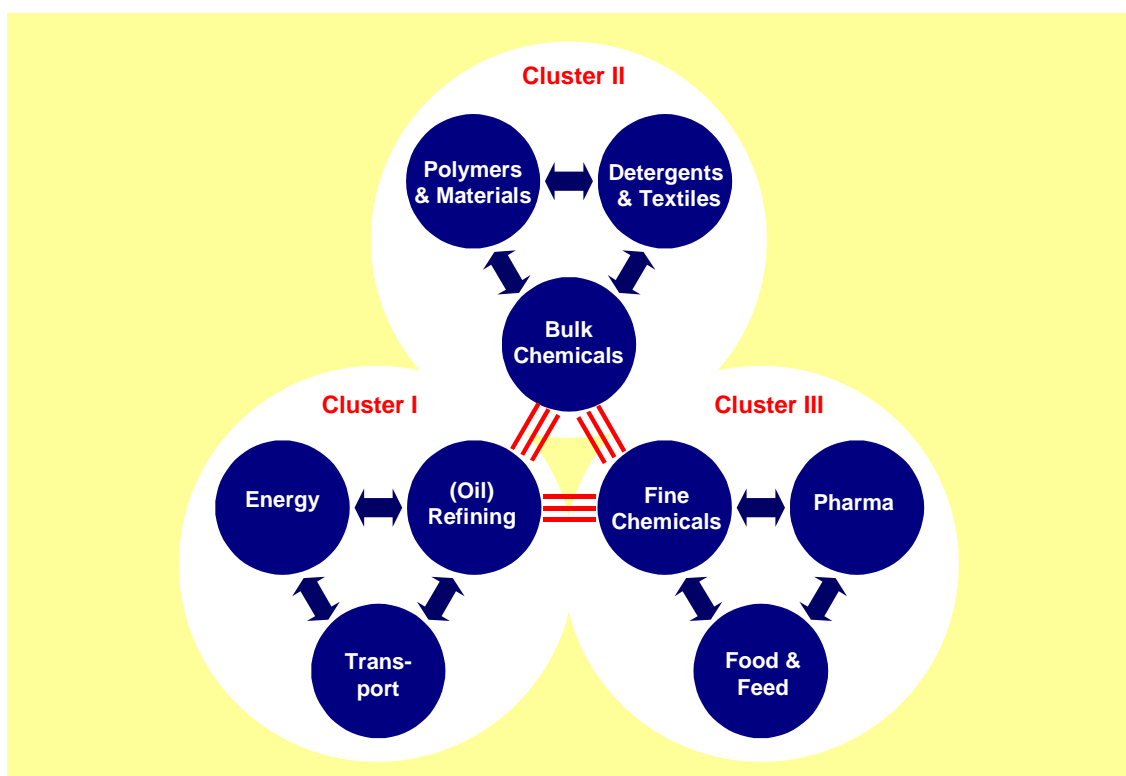
Approach

The use of clusters to capture the relations between relevant sectors and the phased approach are characteristic in the roadmap.

Clusters

Catalysis is widely used in a broad range of industry sectors. For the purpose of the Technology Roadmap Catalysis a clustered approach has been used in order to capture the relations and potential synergies in the catalysis field. The clusters used are:

- **Cluster I: (Oil) Refining, Energy and Transport**
- **Cluster II: Bulk Chemicals, Polymers & Materials and Detergents & Textiles**
- **Cluster III: Fine Chemicals, Pharma & Medical and Food & Feed**



Picture 0.2: Cluster approach used in Technology Roadmap Catalysis

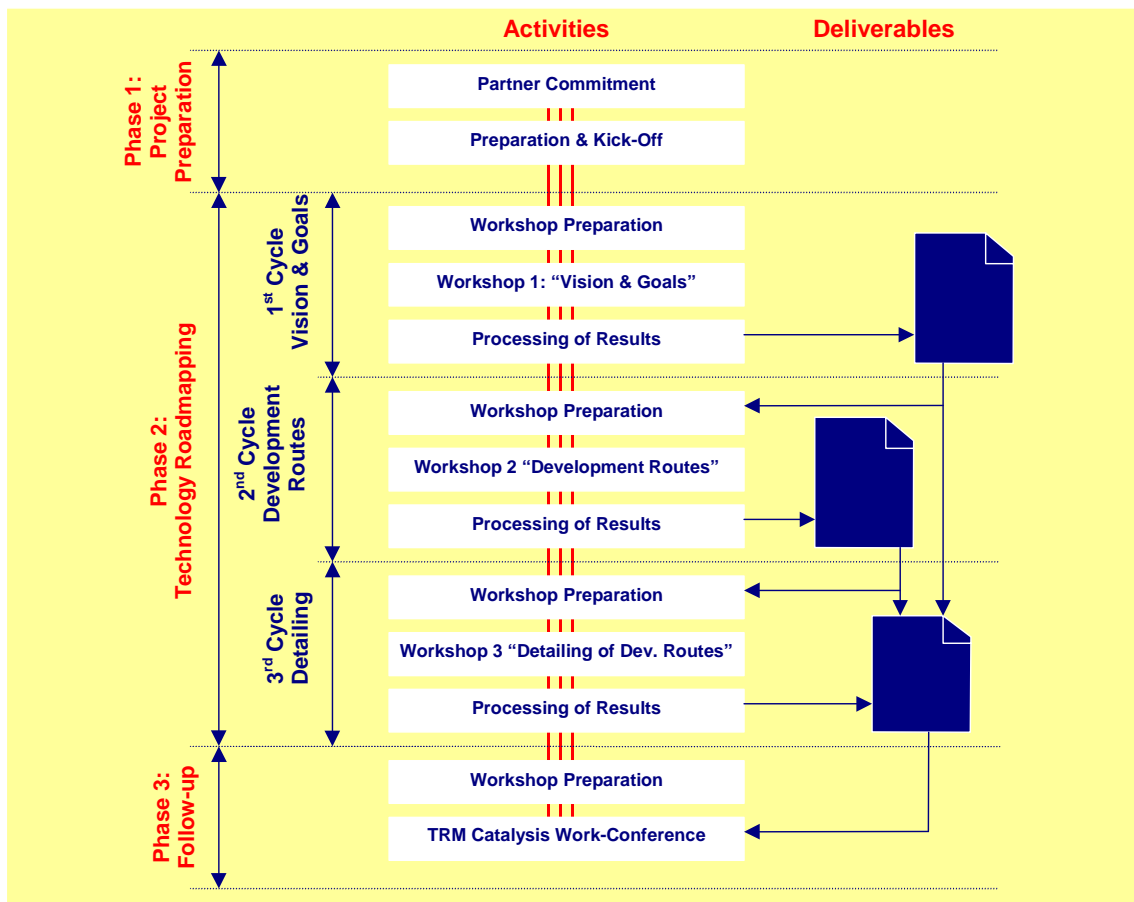
The relations between the clusters and sectors will be covered in the cluster descriptions which can be found in chapters 3 to 5. In these sections the structural relations between the sectors within the clusters and the main relationships between sectors in different clusters will be addressed from the point of view of the respective clusters.

Phased approach

The activities within the roadmap process were divided in three phases.

- **Phase 1: Project preparation** was aimed at securing commitment of all partners involved and at defining an approved approach for the TRM catalysis process.
- **Phase 2: Technology roadmapping** has provided the content of the Technology Roadmap Catalysis through a series of workshops and substantial efforts of the TRM Core team.
- **Phase 3: Follow-up** was aimed at dissemination of the TRM catalysis results and elaborate discussion on future co-operation in the field in order to secure implementation.

The general approach used in the Technology Roadmap Catalysis is shown in picture 0.3.



Picture 0.3: General approach Technology Roadmap Catalysis

Phase 1: Project Preparation

Activities in the first phase of the TRM Catalysis project were:

- a. **Partner Commitment:** During July, August and September 2000 PricewaterhouseCoopers N.V. interviewed key persons of approximately 20 organisations relevant to the field of catalysis and active within The Netherlands¹. During these interviews the commitment to participate in the development and implementation of the TRM-Catalysis as well as identification of relevant overall future trends and developments in catalysis were established. These actions resulted in the installation of the Sounding Board and a Core Team with representation from industry, knowledge infrastructure and government.
- b. **Preparation & Kick-Off:** At the end of August and beginning of October 2000 the Sounding Board and Core Team gathered for the first time. During these meetings the project methodology and approach were discussed, resulting in an approved approach and go-ahead for phase 2 of the TRM-Catalysis project.

Phase 2: Technology Roadmapping

Activities in the second phase consisted of three cycles of workshops aimed at generating content for the catalysis roadmap itself as well as improving communication, building the catalysis network and generating consensus within the field of catalysis in The Netherlands.

Activities in the second phase of the TRM-Catalysis project were:

- a. **1st Cycle "Vision & Goals":** Aimed at generating a joint vision on catalysis in the year 2010 and distillate shared high-priority goals.

Key activities were:

- **Workshop Preparation.** As input for the "Vision & Goals" workshop during October and November 2000 the TRM Core team and PricewaterhouseCoopers N.V. prepared "sector matrices" in which a sector definition, description of the sector in 2010 including the driving forces for developments, sectoral goals with quantification (if possible) and a preliminary identification of the goal related catalysis technologies were included. The sectors used are: Oil refining, Energy, Transport, Environment, Bulk Chemicals, Polymers & Materials, Fine Chemicals, Pharma & Medical, Agro, Food & Feed, Detergents and Textile-Leather-Paper & Pulp. A preliminary "Technology Classification" was also made, capturing technologies relevant for Catalysis.
- **Workshop "Vision & Goals".** The "Vision & Goals" workshop was held on 23 November 2000. Approximately 50 persons from industry, knowledge infrastructure and governmental organisations participated. This workshop was used to validate and further develop the sectoral visions and related R&D goals and to set joint priorities in these goals. This resulted in a set of high-priority goals for each of the identified sectors and the clustering of the sectors in three main areas.

¹ The Dutch Ministry of Economic Affairs also conducted a broad scan of interest in the field of catalysis before starting with the TRM-Catalysis initiative.

- **Processing of results.** The workshop discussions and results were processed and incorporated in updated sector matrices and technology classification and they were subsequently discussed with the Sounding Board.

- b. 2nd Cycle "Development Routes":** Activities in the second cycle of the TRM Catalysis project were aimed at identification of possible development routes which would lead to achieving the high-priority goals as specified in the 1st "Vision & Goals" cycle.

Key activities were:

- **Workshop Preparation.** As input for the "Development Routes" workshop the TRM Core Team and PricewaterhouseCoopers N.V. prepared "Goal related Development Routes" during December 2000 and January 2001 for each of the clusters and their comprising sectors. Based on high-priority sectoral goals (defined in the "Vision & Goals" Workshop and subsequent core team efforts) related products/processes were established and possible technological developments (related to Catalysis) were identified by which the goals could be reached. Where possible, these development routes have been depicted in graphic representations with milestones through time.
- **Workshop "Development Routes".** The workshop "Development Routes" was held on 11 January 2001. Approximately 50 persons from the industry, knowledge infrastructure and governmental organisations participated. This workshop was used to validate and further develop the goal development routes prepared by the core team. Each of the identified clusters and sectors has been discussed in detail. In additional parallel sessions concepts for future co-operation within the field of Catalysis were identified and detailed.
- **Processing of results.** The workshop discussions and results have been processed and incorporated in Cluster documents and a document describing possible concepts for future co-operation by the core team. These have subsequently been discussed with the Sounding Board.

- c. 3rd Cycle "Detailing of Development Routes":** Activities in the third cycle of the TRM Catalysis project were aimed at further (technical) detailing of the development routes identified in the 2nd "Development Routes" cycle.

Key activities were:

- **Workshop Preparation.** As input for the "Detailing of Development Routes" workshop, the TRM Core Team and PricewaterhouseCoopers N.V. have prepared updated cluster/sector documents detailing the identified development routes.
- **Workshop "Detailing of Development Routes".** The workshop "Detailing of Development Routes" was held on 15 March 2001. Approximately 50 persons from the industry, knowledge infrastructure and governmental organisations participated. This workshop was used to validate and further develop the cluster documents describing development routes as prepared by the core team. During the morning session it was concluded that the documents provided a good overview of goal related development routes to the level of detail needed for the TRM purpose. Based on this conclusion it was decided to use the afternoon sessions to discuss general themes and possible concepts for co-operation within Dutch catalysis.

- **Processing of results.** The workshop discussions and results have been processed and incorporated in up-dated Cluster documents and an overview of the discussions on future co-operation as held in the workshop. During the process of writing this TRM Catalysis report the core team had multiple meetings. A “Technology Review Panel” with technology experts was held to check the inclusion of relevant technology-push developments and to provide a second opinion on the cluster descriptions and development routes.

The overall results from the 2nd TRM Catalysis phase have been reported in this document.

Phase 3: Follow-up

Activities in the third phase are aimed at broad dissemination of the TRM Catalysis results as described in this report and at having elaborate discussions on future co-operation in the field.

This will to lay the groundwork for:

- Real implementation and continuous updating of the joint challenges and goals as defined in this Roadmap;
- A strengthened catalysis network and enhanced collaboration between industry and universities in The Netherlands.

In doing so Catalysis within The Netherlands will be able to address and meet the ambitious future demands in an international arena.

Activities in this phase of the TRM Catalysis project were:

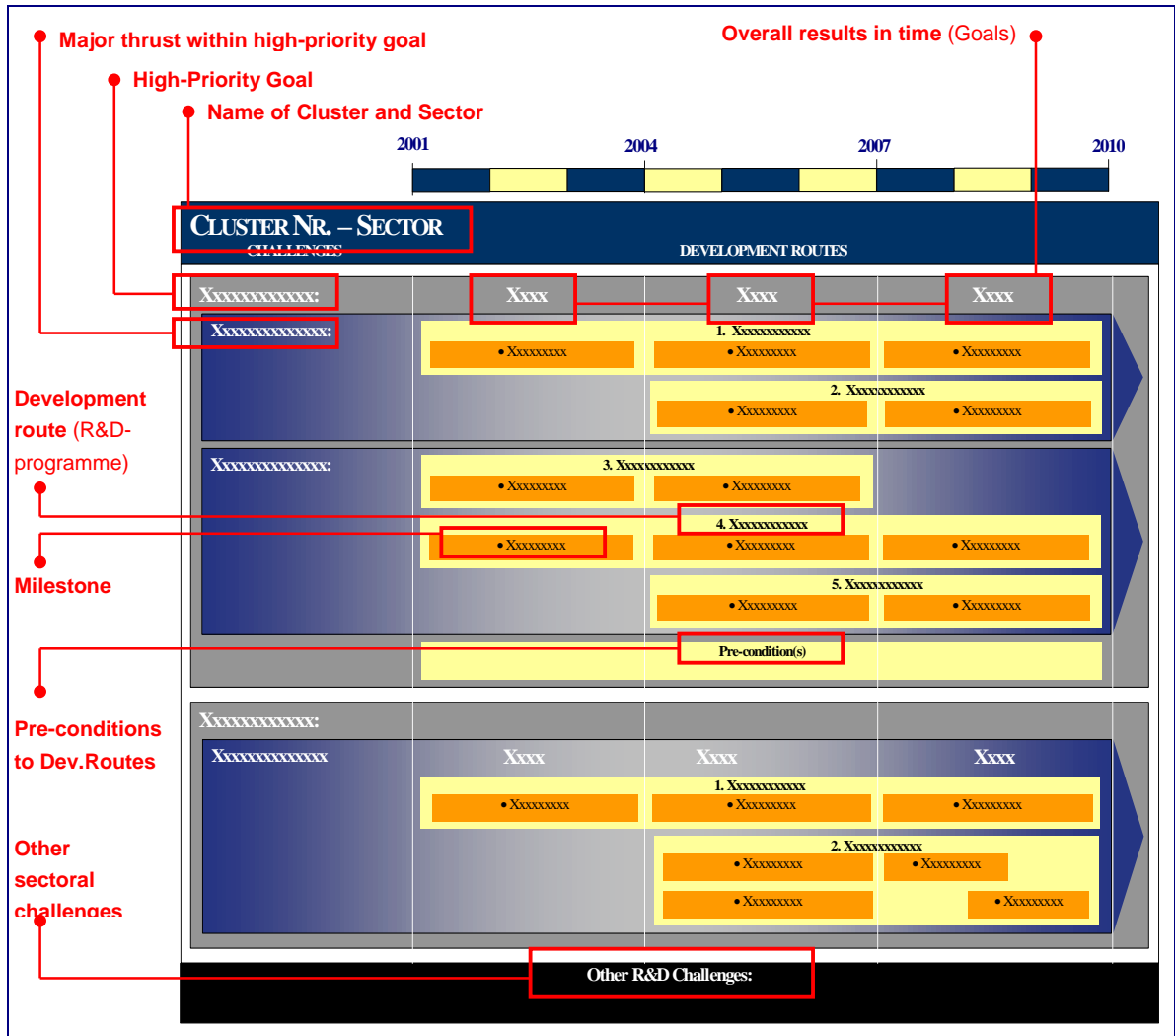
- a. Work Conference Preparation:** As input for the work conference, the TRM core team and PricewaterhouseCoopers N.V. prepared updated cluster/sector documents detailing the identified development routes as part of this TRM Catalysis report (see chapters 3 to 5) and prepared a framework to structure the discussions on future co-operation.
- b. Work Conference:** was held on 7 June 2001 in Nunspeet. Approximately 90 persons from the industry, knowledge infrastructure and governmental organisations participated. The programme consisted of:
 - Presentations of the overall key challenges and the details of the TRM Catalysis at the cluster level in the morning;
 - Discussions on the implementation of the TRM Catalysis through broad co-operation in the field of catalysis in The Netherlands in the afternoon.
- c. Complete the TRM Catalysis report:** Based on the Work Conference of 7 June and feedback from the conference participants, Core Team and Sounding Board the DRAFT Final TRM Catalysis report was updated and finalised and published in July 2001.

Guide to Development Route Graphs and Technology Tables

The high-priority goals have been translated in development routes which provide an overview of routes by which the goals could be achieved. An overview of these development routes are provided in “Development Route Graphs” and the technical details in “Technology Tables”.

Development Route Graphs

The picture below provides a guide on how to read each of the Development Route Graphs.



Picture 0.4: TRM Catalysis Development Route Graph

- **Name of Cluster and Sector:** The cluster and sector to which the development routes belong;
- **High-priority Goal:** The main challenge addressed by the development routes;
- **Major thrust:** Refers to main fields of interest within the specific high-priority goal;
- **Overall results in time:** Main results achieved through the development routes. Results can be depicted at the “high-priority goal” or “major thrust” level;
- **Development Route:** Main R&D programmes needed;
- **Milestone(s):** Result(s) achieved within the development route over time;
- **Pre-conditions:** Elements with impact on development route;

- **Other sectoral challenges:** Goals within the sector in which catalysis could contribute but which are not labelled as high-priority in the workshops.

Technology Tables

Much effort has been put in generating a technology classification which could serve as a generic framework of catalysis-related technologies. The framework (see Annex) consists of three main technology categories: Catalysis Technologies, Process and Reactor Technologies and Scientific Methodologies. Each category has a sub-classification in technology fields and a non-exhaustive examples.

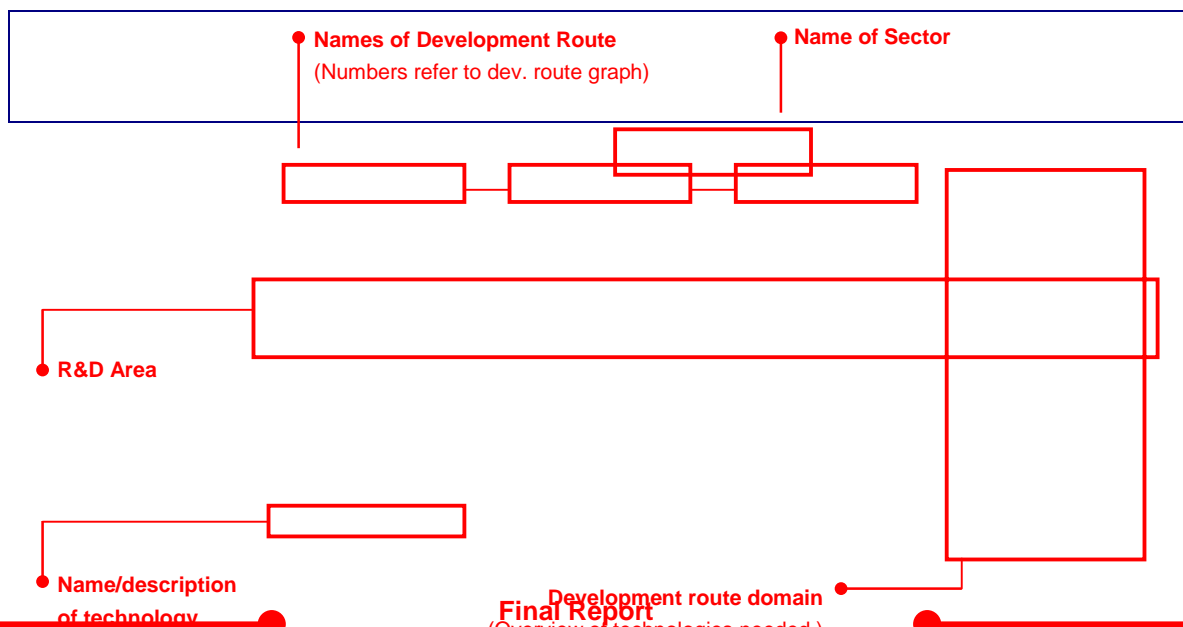
The technology classification at the technology field-level proved to be too generic to be used for the detailing of development routes. The technology classification at the example level proved too long, non-exclusive and too detailed to serve as a general framework in the detailing of development routes. As a consequence, an approach was developed using “R&D Areas”.

The R&D Areas used in the technology tables are:

- **Catalyst design and discovery:** Discovery and subsequent development of (novel) catalysts;
- **Catalyst production:** (Commercial) production of specified catalysts in sufficient quantities;
- **Process design:** Development of new catalytic processes;
- **Process engineering:** Plant design/engineering and realisation;
- **Process monitoring and control:** Monitoring and control of chemical reactions and plant operations.

These R&D areas have a strong interaction with each other. Some sequentiality can be expected but it is not a given as much of the R&D efforts will be in parallel. It is recognised that in order to be successful in any of these R&D-areas, the scientific base as well as basic skills and tools should not only be maintained but improved in specific areas. In general these basic skills are physical, inorganic and organic chemistry with respect to synthesis of materials; analytical tools required to characterise catalytic materials, especially those that enable investigation of catalysts under reaction conditions, i.e. in-situ spectroscopic analysis techniques and catalyst testing including high speed screening, modelling and computational chemistry.

The following illustration provides a guide on how to read the technology tables in this report.



XXXXXXXXXX			
1. XXXXXXXX	2. XXXXXXXX	3. XXXXXXXX	4. XXXXXXXX
Catalyst Design & Discovery			
- XXXXXXXX	- XXXXXXXX	-	- XXXXXXXX
- XXXXXXXX			- XXXXXXXX
Catalyst Production			
- XXXXXXXX	- XXXXXXXX	- XXXXXXXX	- XXXXXXXX
		- XXXXXXXX	- XXXXXXXX
Process Design			
-	- XXXXXXXX	- XXXXXXXX	- XXXXXXXX
Process engineering			
-	-	- XXXXXXXX	-
Process Monitoring & Control			
- XXXXXXXX	-	- XXXXXXXX	- XXXXXXXX
		- XXXXXXXX	- XXXXXXXX

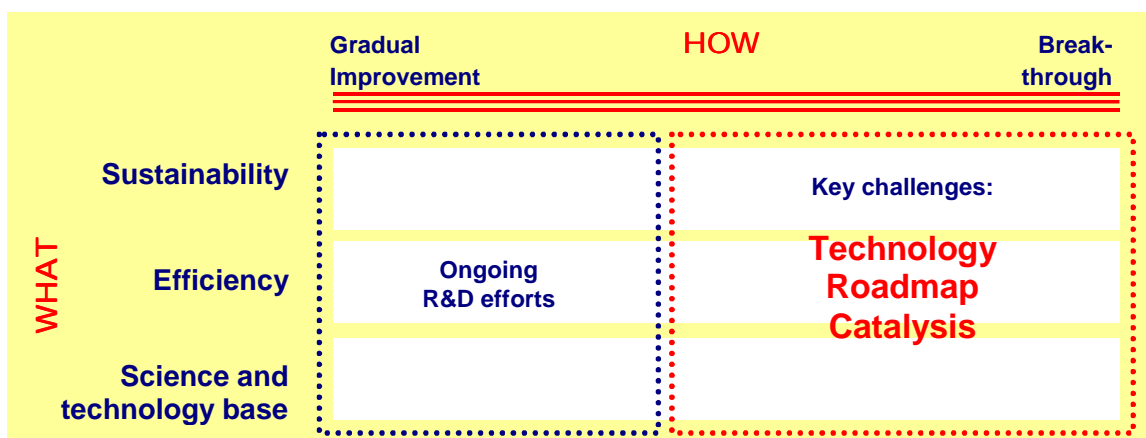
Picture 0.5: TRM-catalysis technology table

- **Name of Sector:** The sector to which the depicted development routes and related technologies belong;
- **Names of Development Route:** Listing of development routes as identified in the development route graph. The numbers provide direct reference.
- **R&D Area:** Relate to the R&D areas as described above.
- **Name/description of technology:** Name and/or description of the specific critical technologies for a specific development route within the R&D Area.
- **Development Route Domain:** Overview of all critical technologies needed within the development route.

2. KEY CHALLENGES FOR CATALYSIS

Within the setting of this technology roadmap and based on the discussions and insight generated in the workshops by the core team and Sounding Board some key challenges for the catalysis field have been identified. These challenges are generic and of major importance to the whole field catalysis in The Netherlands and focus on the “**how**” and “**what**” of catalysis R&D.

- a. The “**HOW**” relates to the focus in the execution of the catalysis-related activities ranging from gradual improvement to **breakthrough** in which creating breakthroughs poses the real challenge.
- b. The “**WHAT**” refers to the challenges which direct the activities within catalysis, being:
 - **Sustainability**
 - **Efficiency**
 - **Science and technology base**



Picture 2.1: Key challenges in Catalysis

Breakthrough approach

The gradual improvement of existing technologies, products and processes is of course very important in catalysis-related R&D. The gradual improvements however are adequately covered by existing ongoing R&D efforts and interests in the catalysis field.

Creating breakthroughs through systematic innovation by exploiting the potential of catalysis on an integrated, broad scale on the other side, is key to further develop and exploit the international position of Catalysis within The Netherlands. Such a focus is actively advocated in this technology roadmap as it requires additional attention and efforts to create such breakthroughs. This means not only setting of joint priorities in terms of technological goals and projects but also stimulating a culture fostering changes, innovation, enthusiasm and surprise.

Towards this aim “**integration**” and “**systematic**” are considered to be conditional requirements.

Integration

Integration within the context of this Technology Roadmap relates to:

- **Integration of Industry and knowledge infrastructure:** In order to achieve optimal synergy in industrial and university research and development, the co-operation should be improved in a structural way.
- **Disciplinary Integration:** In order to achieve real breakthroughs in catalysis R&D integration of all related technological fields is needed in identifying and solving catalysis-related problems. This relates not only to integration of the fields of homogeneous, heterogeneous and bio-catalysis but also to disciplines such as reactor design and (plant) engineering, materials science, biology, etc.
- **Integration in areas of application:** Integration is also needed on the application side of catalysis. In achieving breakthroughs substantial R&D efforts are needed sometimes with high related costs and risks. Integration is essential in order to achieve shared costs and risks, application of new catalysis technologies in the broadest way possible and cross-fertilisation in R&D.

Systematic

Systematic within the context of this Technology Roadmap relates to the fact that the R&D-efforts should be aimed at shared goals and collaboration towards these goals. This roadmap provides a framework of shared goals in the field of catalysis both at the generic catalysis level (the “what” as described below) and at the cluster-level (as described in chapters 3 to 5).

Sustainability

Catalysis is essential for the development of a sustainable world and is a key technology in achieving the sustainability goals.

The impact of catalysis on sustainability is broad and diverse but is directly related to the three key characteristics of the technology. Being:

- **Selectivity** (the ability to accelerate only specific, desired reactions) is directly related to the development of new routes for new and existing products as well as the reduction of waste in a broad sense. Catalysis plays a key role in reduction of by-products in the synthesis of desired products (waste prevention), effective transformation of undesired waste streams (clean-up and recycling), efficient and flexible use of feedstocks.
- **Activity** (the impact on the reaction rate) is directly related to the use of energy and processing time. Application of catalysis and improved catalytic activity in specific processes helps to reduce the overall energy needed to manufacture desired products.
- **Stability:** The ability to maintain selectivity and activity during extended periods of processing. Improved catalytic stability will ensure that the use of catalysts themselves will not result in new large waste streams.

The nature of catalysis is such that these three characteristics of catalysis have remained and will remain a focus in all catalysis-related research and development activities towards sustainability in a broad range of sectors, products and processes.

The impact on the sustainability of specific societal and industrial needs and the related products and processes is generic to all three clusters and comprising sectors in this technology roadmap. Details on the sectoral impact can be found in the cluster descriptions. In many areas, and especially reduction of waste and energy use, legislation will be a major driver which this roadmap has not specifically addressed as developments in this area are difficult to predict.

Efficiency

Efficiency is a main driver in catalysis related R&D as it has a direct link to the maximisation of the benefits (desired products, profit, etc.) with a minimum of costs in a broad sense (e.g. environmental impact, materials use, energy, capital investment, etc.).

Efficiency is addressed at three levels:

- **Atom-efficiency:** Improving efficiency in the use of scarce resources through steep reduction of waste and use of raw materials. Catalysis does impact the effective use of available feedstocks.
- **Cost-efficiency:** Catalysis has significant impact on cost-efficiency through improved reaction effectiveness (e.g. reduced separation and waste disposal costs), reduced capital investments (e.g. novel process and reactor concepts), improved plant and feedstock flexibility, reduction and production time, etc.
- **Energy-efficiency:** Key element in the use of catalysis is the ability to reduce the energy needed to manufacture desired products and operate specific processes.

Key challenge for catalysis is to apply its potential towards the further and significant improvement of efficiency which will benefit the end user through better and cheaper products and processes, the environment through sustainability improvements and the industry through increased profit margins.

Science and Technology Base

The science & technology base within universities, knowledge and industry is the foundation for the future catalysis R&D. Maintaining the strength of the science & technology base and its long-term international development with focus on interdisciplinary cross-fertilisation is crucial.

The current developments of reduced industrial (corporate) R&D and a shift towards short-term applied R&D as well as the trend towards reduced numbers of students in the technical disciplines at universities need to be addressed to maintain the current science & technology bases in The Netherlands. All organisations (industry, knowledge infrastructure and government) need to be actively involved in this key challenge in order to secure the future of the catalysis science and technology base.

3. CLUSTER I: (OIL) REFINING, ENERGY AND TRANSPORT

Introduction to Cluster I

Cluster I consists of the sectors energy, transport and refining. It is concerned with sustainable development of energy and mobility, including conversion of (renewable) energy carriers, storage (especially of hydrogen) and reduction of emissions accompanied by energy and mobility.

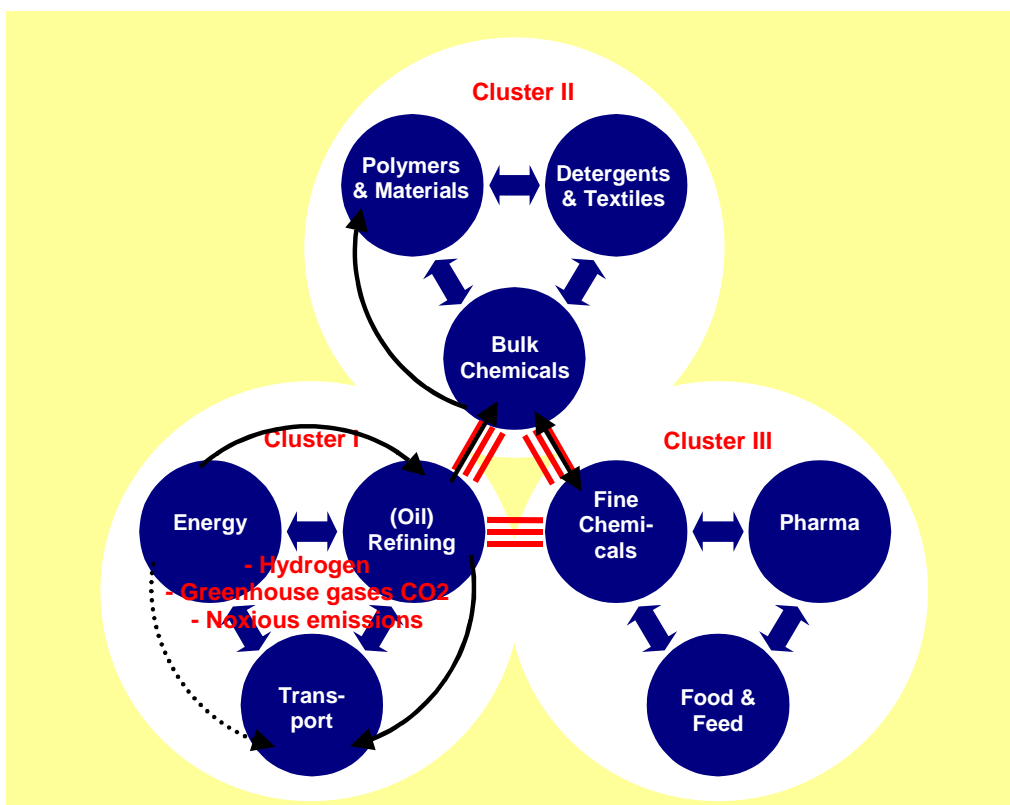
Typical for this cluster is that the products are relatively constant with respect to composition and variations are more often due to external factors than to technology “push”. That is different from e.g. new detergents and pharmaceutical products, which are generated in periods of months or a few years driven by innovation. Energy carriers remain the same (electricity) or change gradually; like the user’s ratio of oil/coal to gas because of availability and cost. In addition, process innovations in this cluster have a long lead time and require external push; i.e. catalytic converters to clean emissions from cars have been a technology breakthrough but it took 10-15 years (the lifetime of existing cars) to be fully effective in combination with tax incentives for the use of unleaded petrol. A third difference with the other clusters is that product cost is a key item. Value generation by product differentiation (standard in food, pharmaceutical and detergent sectors) is a difficult marketing tool when it comes to fuels and other energy carriers. Therefore a technology push is often not sufficient enough to introduce new products; for example low sulphur (<50 ppmw) diesel is currently introduced in view of future legislation (2005 specification) whereas the technology is already in place to produce < 1 ppmw S but it is not generally used because of costs.

Technology push will have an impact on areas such as hydrogen technologies, nano-technologies, photo-synthesis/solar technologies and materials. However, legislation, public opinion and economical incentives will drive “investment” decisions in new technology developments (Catalysis versus IT?), and which determine technological breakthroughs will cross the threshold of widespread commercial application. On the other hand, the long lead-time of implementations towards a sustainable society in the area of this cluster, requires development of the science & technology basis to already start now in order to be effective this century.

Relations between the sectors

The relations between the sectors within cluster I are strong (see picture I.1.) and result in a set of “General Themes” (items which occur throughout the sectors within the cluster). These general themes are:

- **Hydrogen** production, storage, and handling;
- **Noxious gaseous emissions** - emissions can be regarded as a general theme over all clusters;
- **Greenhouse gases** like CO₂ in relation to global warming.



Picture I.1: Relations between sectors as seen from a cluster I-perspective.

A description of the general “cross-sector” themes within cluster I, and of the sectors energy, refining and transport will be discussed below. This is followed by a description of the various short-term and long-term research goals related to catalysis within each sector and the development routes in order to achieve these goals.

Roadmap General Themes

The general themes in cluster I are Hydrogen, Gaseous Noxious Emissions and Greenhouse Gases. These themes will be detailed below.

Description and challenges in General Themes

Hydrogen:

Theme Description: Hydrogen is considered to be an important “fuel” or energy carrier in the near future. The theme is considered very relevant in a sustainable energy and mobility development as hydrogen is considered one of the key energy carriers in terms of energy source, as fuel for transportation and as intermediate in the conversion of renewable energy sources. Existing processes for hydrogen production are currently related to the refining sector. In addition to its role as energy carrier, hydrogen is also of relevance for the production of cleaner fuels. The latter will require a growth of around 20% to fulfil the expected legislation demands. Small-scale hydrogen production for mobile applications is covered under the Transport sector. A complete hydrogen economy is not expected in the next decades. However, developments have started already. Expectations are that, in 2010 hydrogen production on a refinery scale will have increased by at least 100%, to meet emission legislation and to provide hydrogen as a fuel. Moreover, the reduction in aromatics in fuel has resulted in lower severity of naphtha reforming which is compensated for by additional methane reforming capacity. The use of hydrogen as a transportation fuel has been demonstrated (both hydrogen fuelled cars and hydrogen manufacturing “on board”).

Theme Challenges: Hydrogen production in the refinery conventionally uses naphtha reforming. Because of the decreasing amount of aromatics allowed in fuels, the relevance of this technology for hydrogen manufacturing will decline. Thus, at the same moment that demand for hydrogen increases considerably, alternative sources of hydrogen will have to be found on the short term for refining processes. For fuels production, altogether new technologies will have to be developed to commercial viability. Methane is the fossil fuel with the highest H/C ratio, so it is the obvious first choice for the production of hydrogen using technologies close to conventional. At a later stage, water is the obvious starting material in combination with a renewable energy source. The current hydrogen production is equivalent to only about 3% of the total energy consumption at the moment. Energy losses for hydrogen production from fossil fuels are projected to be considerable. Storage and recovery of hydrogen also requires significant amounts of energy. However, economic considerations will probably support the initial development of processes based on fossil fuels. Overall, lead times for total transfer to hydrogen as energy carrier will be long. Another challenge related to hydrogen production and the introduction of fuel cells on the market is the search for new membrane materials for proton-exchange-membrane fuel cells. These new developments in polymer materials are part of the activities of cluster II.

In addition to these technical challenges, hydrogen has an image problem with respect to safety (Hindenburg disaster in 1936, “knalgas” reaction as demonstrated in high-school chemistry). The launch of hydrogen as a large-scale fuel will have to deal with this initial scepticism. Given the

existing safe technology for handling hydrogen at high pressures in industry, as well as the commercial (now obsolete) distribution of town gas, the scepticism should decrease rather fast. However, any accidents in the first stages of implementation may dramatically affect the ease of market introduction and thus much attention has to be given to good public relations.

Gaseous Noxious Emissions

Theme description: Historically, minimising the production of undesirable by-products has been one of the drivers of catalysis, generally known as product selectivity. This is still a current issue for all sectors discussed in this technology roadmap. Cluster I limits itself to gaseous emissions as undesirable by-products (i.e. it does not include solid/liquid waste). In this respect, selectivity as part of catalysis is only of limited interest. This is because vapour emissions are either a result of feed properties (like sulphur content in fuel resulting in the emission of SO₂) or process conditions (high temperature resulting in the formation of NO_x from molecular nitrogen and oxygen present during combustion); therefore not a result of an undesired catalytic reaction. However, catalysis plays an important role in pre- and post-treatment processes. It was considered useful to deal with emissions, from both mobile and stationary sources, as a separate item instead of repeating goals and technologies for each of the individual sectors discussed above. For 2010 we expect a further reduction in emissions as a result of improved catalyst technology and more stringent legislation with respect to fuel properties.

Theme challenges: Society desires chemical processes with zero emissions and zero by-product formation. This is a major challenge, not only for catalyst technology, but also economically. Adverse economics often hinder the commercial development of interesting emerging technologies. Thus, the implementation of further stringent legislation will be of key importance for such technologies to appear on the market.

Greenhouse Gases

Theme description: CO₂ formation is an inherent consequence of the use of oxidation processes using hydrocarbon feeds, such as combustion (complete oxidation) for the production of heat and power in the use of transportation fuels, and (selective) partial oxidation processes for the production of bulk and fine chemicals. A substantial CO₂ reduction can only be achieved by more efficient fossil fuel consumption and catalysis can play a role in more selective partial oxidation.

Theme challenges: Methods need to be found to minimise CO₂-emission, i.e. process intensification/efficiency or CO₂-capture technologies. Advanced nitrogen-oxygen separation technologies enable oxidation of hydrocarbons with pure oxygen with the additional advantage that CO₂ in a concentrated flue-gas can be sequestered more efficiently. Hydrogen manufacturing using pure oxygen is also associated with concentrated CO₂. Alternatively, catalysis can play a role in (1) concentration and sequestration of C/CO₂ and (2) the development of catalytic systems, as a result of which CO₂ can be converted to useful organic molecules. For the latter, inspiration can be found in biological systems and, as a consequence, efforts will have to be made to mimic photosynthetic systems for the conversion of CO₂ to e.g. sugars. Sequestration of C/CO₂ can be considered a boundary condition for sustainable development in a hydrogen-based economy using fossil fuels. Solutions have to be evaluated on technological and economic viability.

Overview high-priority goals

Based on the “Vision & Goals” workshop a set of goals (including quantification where possible) were defined. The high-priority goals are:

- a. **High-priority goal 1: Hydrogen General Theme:** The Hydrogen general theme as related to catalysis consists of three major challenges. These are:
 - **High-priority goal 1a - Increased Hydrogen Production:** Hydrogen production without parallel production of CO₂. Naphtha reforming and the obvious replacements using methane or gasification of residue will always produce oxidised carbon in some form (CO or CO₂). Therefore, sustainable hydrogen production from fossil fuels must be accompanied by CO₂ sequestration. Alternative technologies could start from water using a renewable energy source.
 - **High-priority goal 1b - Improved Hydrogen Storage Capacity:** The target is to develop a storage system that will allow cars to drive with the same range of about 500 kilometres per tank. This translates to storage capacity descriptors for both weight and volume percent. In addition to the use of the new system should be very similar to present experience. That means for instance that fuelling a car should be fast and convenient (response time of the storage system is crucial here) and the storage system in the car should allow similar performance of the car (e.g. in terms of acceleration).
 - **High-priority goal 1c - Improved Hydrogen handling:** Improve energy efficiency of storage and retrieval. Storing hydrogen either under pressure or in a hydride costs energy, and so does retrieval. The objective is to minimise these losses. The requirements on performance parameters described under storage, i.e. the new system mimicking present practice also hold here.
- b. **High-priority goal 2: Noxious Gaseous Emissions:** The ultimate dream and thus a long-term goal is zero emission. Important noxious gaseous pollutants are SO_x, NO_x, soot, VOC and chlorinated (aromatic) hydrocarbons. Other important gaseous emissions, known as greenhouse gases, are CO₂ and N₂O. Different levels of reduction can be put forward for the noxious pollutants, whereas a clear development option for catalysis in relation to greenhouse gas emission reduction has to be defined in a separate R&D programme. The ambitious overall goal of zero emission can unfortunately not be reached by the year 2010 and intermediate high-priority goals have to be defined. They are as follows:
 - **For stationary sources**, such as refineries and waste-to-energy plants, a 90% reduction for SO_x, 90% decrease for NO_x and for chlorinated (aromatic) hydrocarbons below ppb levels is expected.;
 - **For mobile sources**, the VOC and benzene emissions have to be decreased by 80% (in comparison with the 2000 level). For NO_x and soot a 80% and 90% reduction, respectively, has to be implemented.

- c. High-priority goal 3: Greenhouse gas emissions:** The role of catalysis in CO₂ sequestration is limited: catalysis deals with increasing chemical reaction rates along the most desirable path: CO₂ is already the most desirable product to release the chemical energy in a hydrocarbon molecule and the oxidation reaction involved is often a non-catalytic reaction. The current role of catalysis in sequestration of CO₂ produced in the energy-mobility cluster is virtually zero. However, if CO₂ sequestration by chemical reactions (e.g. to form carbonates) is considered a viable option, catalysis can play a role in increasing preferred reaction rates as in any other area. To a limited extent catalysis can play a role in more selective catalytic partial oxidation processes, especially in the bulk chemicals area.

Catalysis might play, however, a significant role in the reduction of CO₂ emissions with the introduction of renewable energy sources (sunlight). This allows the production of valuable chemicals, like methanol, as listed under the energy sector. Separate research programmes on photosynthesis enzyme mimics are of great importance in this respect. Although CO₂ sequestration is listed as a general theme for this TRM-Catalysis, it is not considered useful to list a separate goal for reduction of CO₂ emissions in relation to catalysis because CO₂ sequestration is essentially a physical, non-catalytic process. However, catalysis can be relevant in CO₂ capture, concentration and/or separation.

Development Routes General Themes

Picture I.2 provides an overview of the General themes: Hydrogen and Reduction of Gaseous Noxious Emissions development routes.

2001 2004 2007 2010

CLUSTER I – GENERAL THEMES		DEVELOPMENT ROUTES	
CHALLENGES			
Hydrogen:			
Hydrogen Production	60% increase in hydrogen production without additional CO ₂ emission		
	1. Catalytic Naphtha reforming • continuous improvement		
	2. Catalytic reforming of methane 3. Gasification of residue • Demonstrate in combination with CO ₂ sequestration		• Hydrogen plant with CO ₂ sequestration
	4. Catalytic Partial Oxidation • Demonstration unit	• Commercial units	
	5. Cracking of hydrocarbons to carbon residue and hydrogen • proof of concept and pilot plant		• Demonstration unit
	6. Gas to liquids and hydrogen • proof of concept		• Pilot plant
	7. Renewable bio-mass transformation • proof of concept		• Pilot plant
	• (Proof of concept)	8. Electrolysis on renewable sources • Pilot plant	• Commercial unit
	9. Thermal dissociation • Roof of concept		
			10. Bio-dissociation (bacteria & sun) • Proof of concept
Hydrogen Storage	5% m H ₂ 1. High Pressure / Low Temperature • Demonstration unit	7,5% m H ₂ • Market introduction	10% m H ₂
	• (Proof of principle)	2. Adsorption of hydrogen on carbon • Proof of principle in demonstration unit	• Market introduction
	3. Use of Metal Hybrides • Proof of principle		• Demonstration unit
	4. Use of Redox couples • Proof of principle		• Demonstration unit
Hydrogen Handling	Recovering 90% of the energy stored		
	1. New materials • Ongoing research		
	2. Fundamental sciency & supportive technology • Ongoing research		
Reduction of gaseous noxious emissions:	80 - 90% reduction of noxious gaseous pollutants		
Development routes:	1. Improved SO ₂ abatement from stationary sources • Proof of concept		• Technology demonstrated on pilot scale • Market introduction
	2. Catalytic burner • Proof of concept		• Demonstration unit
	3. SO ₂ resistant materials for NO _x storage (avoid SO ₂ → SO ₃) • Proof of concept		• Demonstration unit
	• (Proof of concept)	4. VOC oxidation at room temperature • Demonstration unit	• Market introduction
	• Proof of concept	5. Development of catalytic filtes as end of pipe solution to remove particulates • Demonstration unit	• Market introduction
	6. Catalysts for reaction of NO with soot • Proof of concept		• Demonstration unit
	• Proof of concept	7. Replacement of noble metal catalysts by transition metal (oxides), carbides, nitrides, lanthanides • Demonstration unit	• Market introduction
			8. NO decomposition catalysss • Proof of concept

Picture I.2: Catalysis in Hydrogen Roadmap (General Themes)

High-priority goal 1a - Increased Hydrogen Production

Hydrogen production for refinery purposes was about 10 million tons per year in 1990. The expected production in 2050 is 50 million tons. This indicates that considerable additional capacity will be required even in the next 10 years.

Development Options are:

a. Short Term:

- Catalytic reforming of naphtha
- Catalytic reforming of methane (followed by watergas shift and CO₂/H₂ separation)
- Gasification of residue (followed by water gas shift and CO₂/H₂ separation)
- Catalytic partial oxidation (CPO) based on natural gas and light hydrocarbons (followed by watergas shift and CO₂(N₂)/H₂ separation)

These options are already commercially demonstrated (first three development options) or about to be demonstrated (the CPO option) but continuous improvements are expected. The major technical hurdle is to combine these options, based on fossil fuel, with CO₂ sequestration.

b. Mid Term:

- Cracking hydrocarbons to carbon residue and hydrogen
- Gas-to-liquids + hydrogen
- Renewable bio-mass as a base for hydrogen production (involves bio-residuum cracking/gasification see sector 'energy')

These three options are in an exploratory/development phase and significant efforts are required to demonstrate that these options are viable on a commercial scale.

c. Long Term:

- Hydrogen production by dissociation of water
- Electrolysis based on renewable energy sources like wind and hydro via electricity or directly by solar conversion: see Energy Sector)
- Thermal dissociation
- Bio-dissociation using bacteria and sunlight

These options require significant scientific and technological break-throughs to be of commercial relevance.

Hydrogen based technology is typically a product of this theme, and therefore an output rather than a required technology. Several development routes listed above are not using catalysis. The stages of technology development for those routes involving catalysis are listed below.

Technologies in Increased Hydrogen Production				
1. Catalytic reforming of naphtha	2. Catalytic reforming of methane	3. Gasification of residue	4. Catalytic partial oxidation	5. Cracking of hydro-carbons to carbon residue and hydrogen
Catalyst Design & Discovery				
- Continuous improvement	- Continuous improvement		- High temperature stability	- Non-catalytic?
Catalyst Production				
			- Noble metal availability	
Process Design				
			- Relevant	- Relevant
Process engineering				
Relevant for all development routes				
Process Monitoring & Control				
- Relevant	- Relevant			

Table I.1: Technological focus of catalysis in hydrogen production

Technologies in Increased Hydrogen Production (continued)				
6. Gas to liquids and hydrogen	7. Renewable bio-mass transformation	8. Electrolysis of water based or renewable energy sources	9. Thermal dissociation of water	10. Bio-dissociation of water using bacteria and sunlight
Catalyst Design & Discovery				
- Very relevant	- Improve existing catalysts			
Catalyst Production				
Process Design				
			- Relevant	
Process engineering				
Relevant for all development routes				
Process Monitoring & Control				

Table I.1(continued): Technological focus of catalysis in hydrogen production

High-priority goal 1b - Improved Hydrogen Storage Capacity

The use of hydrogen as energy carrier in future applications, such as fuel cells, critically depends on methods to store and retrieve hydrogen in a simple and energy-efficient way. Several development options can be envisaged. Goal related development routes are:

- a. High pressure/low temperature
- b. Adsorption on carbon
- c. Use of metal hydrides (e.g. magnesium hydrides and sodium borohydride)
- d. Redox-couples (e.g. emulsions of Na)

Developments will have to start immediately and will have to be part of a continuing programme. It is important that new hydrogen storage materials have a storage density which is significantly higher than that of hydrogen gas at high pressures and low temperatures. Another important issue is the ease of hydrogen retrieval (i.e. speed and required energy input).

Key technologies in the development routes for improved hydrogen storage are materials and material modification technologies, (fundamental) molecular insight (structure and architecture) and electro-chemistry (fuel cell related of technologies. Option is along existing R&D conventional Redox couples in batteries - Philips).

Technologies in Improved Hydrogen Storage Capacity			
1. High pressure/low temperature processes	2. Adsorption of hydrogen on carbon	3. Use of metal hydrides	4. Use of redox couples
Catalyst Design & Discovery			
- Fundamental inorganic chemistry	- Control over carbon properties - Molecular insight in structure and activity	- Safe and reliable	- Materials design
Catalyst Production			
- Relevant	- Relevant	- Relevant	- Relevant
Process Design			
- Reduced energy input	- Reduced energy input	- Reduced energy input	- Reduced energy input
Process engineering			
Process Monitoring & Control			

Table I.2: Technological focus of catalysis in improved hydrogen storage capacity

High-priority goal 1c - Improved Hydrogen Handling

Apart from a high capacity (in terms of mass hydrogen stored per mass adsorbent), also the thermodynamic efficiency, scale up and safety are key, especially related to mobile and small-scale home-based applications; industry has already proved to be able to use hydrogen safely on a large scale. The target is to recover at least a minimum of 90% of the energy stored. This means that the storage-release cycle must become much more efficient than it is now. The materials research required here is related to catalyst research.

Goal related development routes are:

- a. **Materials research** (Hydrides, sponge structures, carbon nanotubes, clathrasils)
- b. **Fundamental supportive research:** Adsorption/desorption kinetics, thermodynamics, water corrosion resistance.

The main R&D areas relevant to these development routes are depicted in the table I.3.

Technologies in Increased Hydrogen Handling	
1. Materials research	2. Fundamental supportive research
Catalyst Design & Discovery	
- Highly relevant	- Highly relevant
Catalyst Production	
- Relevant	
Process Design	
	- Relevant
Process engineering	
Process Monitoring & Control	

Table I.3: Technological focus of catalysis in hydrogen handling

High-priority goal 2 - Noxious Gaseous Emissions

The high-priority goals can be addressed by the following development routes:

a. Prevention of (transport) emission by:

- Development of new/cleaner fuels or use of fuel additives to enable catalytic conversion and sensors, see refining sector- *short-term/medium-term*
- Development of a catalytic burner (used in combination with current engine-technology) - *medium-term*
- Improved engine management by use of sensors and management systems - *ongoing*

b. End of pipe solutions for the above described noxious compounds:

- Development of new selective and waste-tolerant catalysts - *medium-term*
- Development of catalytic filters - *medium-term*
- Development of afterburners and intermediate adsorbents (e.g. NO_x-trap catalysts) - *medium-term*

A boundary condition for catalytic solutions found here is the prevention of N₂O formation.

c. Replacement of noble metal catalysts:

Because of the shortage in noble metals and the expected increase in demand for the catalytic cleaning of gaseous emissions alternatives have to be developed. These alternatives can be based on:

- Transition metals or transition metal oxides - *short-term*
- Carbides/nitrides/lanthanide's - *medium-long-term*

These options are considered for both stationary and mobile power sources.

The technological needs related to these development routes have been divided in the three timeframes.

• Short Term:

- Mobile: SO₂ resistant catalysts
- Avoid SO₂ oxidation to SO₃
- SO₂ abatement: Improved current processes, especially directed towards cheaper, more efficient processes
- Soot abatement: functional integration catalyst development and reactor design
- VOC – oxidation at ambient temperature & pressure

• Mid Term:

- Soot + NO → CO₂ + N₂
- Removal/separation of fine particles (including application of these solids in other areas)

• Long Term:

- NO-decomposition

R&D with respect to soot and NO is part of an ongoing programme that requires integration of various disciplines involved. Obviously there is a link with developments in the transportation sector in that the development of hybrid or fuel cell powered vehicles already result in a significant reduction of emissions.

Technologies in reduction of noxious gaseous emissions			
1. Improved SO2 abatement from stationary sources	2. Catalytic burner	3. SO2 resistant materials for NOx storage (avoid SO2 →SO4)	4. VOC oxidation at room temperature
Catalyst Design & Discovery			
	- New materials	- Improved catalytic systems	- Improved catalytic systems
Catalyst Production			
	- New preparation routes		- Relevant
Process Design			
- Relevant			- Relevant
Process engineering			
- Relevant		- Optimisation process conditions	
Process Monitoring & Control			
		- Sensor development and integration	

Table I.4: Technological focus of catalysis in reduction of noxious gaseous emissions

Technologies in reduction of noxious gaseous emissions (continued)			
5. Development of catalytic filters	6. Catalysts for reaction of NO with soot	7. Replace noble metal catalysts by transition metal	8. NO decomposition catalysts
Catalyst Design & Discovery			
- Better understanding of working principle	- Better understanding of working principle	- Activity at low temp without by-product formation	- Highly relevant
Catalyst Production			
- Relevant	- Relevant	- Novel catalyst preparation conditions	
Process Design			
- Relevant	- Relevant	- Relevant	
Process engineering			
Process Monitoring & Control			

Table I.4(continued): Technological focus of catalysis in reduction of noxious gaseous emissions

Roadmap Energy

Sector Definition and Vision

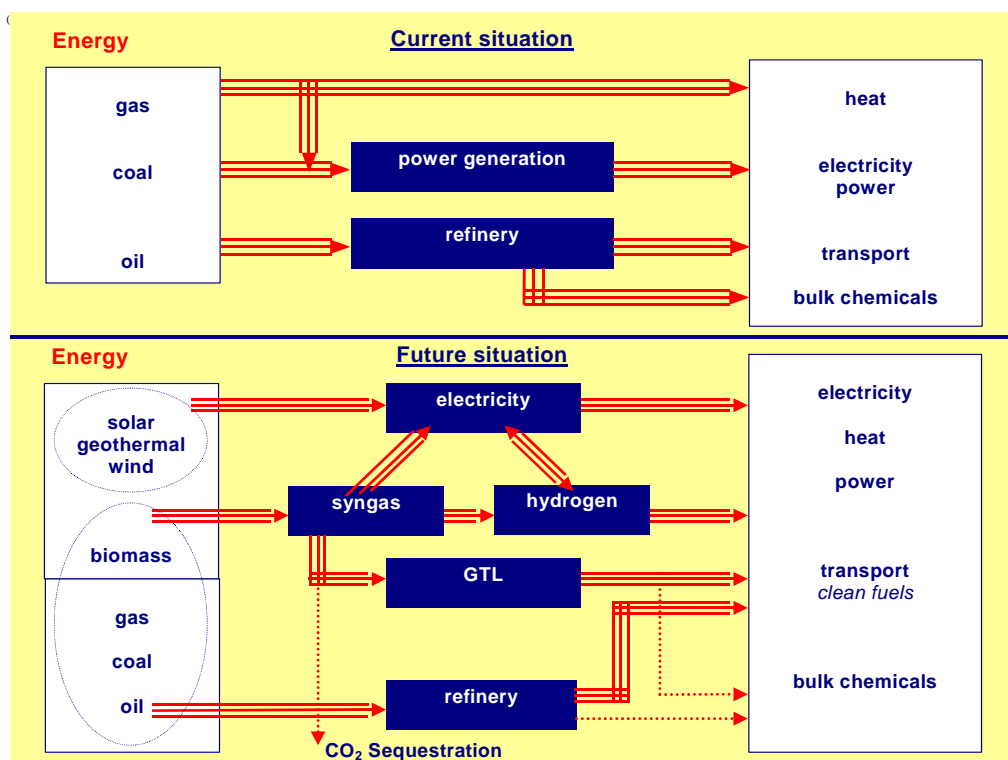
Sector definition:

This sector is concerned with production of energy in the form of electricity or heat, combinations thereof (Combined Heat and Power, CHP) using fossil (oil, gas and coal) or renewable energy sources (solar energy, wind energy, biomass, hydro, etc.) including intermediate energy carriers like hydrogen. Within energy production, catalysis is used as a tool in most cases (part of the toolbox, together with reactor technology etc.). In a sustainable development of energy sources, catalysis will play a role in specific areas.

Description of the sector in 2010:

Global energy demand has increased significantly due to continued growth of the world population and its prosperity. Nationally, the energy demand of The Netherlands stabilised at the level of 2000. Although advances in gas-to-liquids technology have extended the expected lifetime of fossil fuels, renewable energy sources play an ever-increasing role in energy production despite fluctuations in (political) perceptions. In 2010 the best (mix of) technique(s) for sustainable energy supply will be identified. Biomass conversion and waste-to-energy using modern high-performance ovens has become state-of-the-art, enforced by legislative measures and constraints to waste handling and emission reduction (e.g. dioxins and PCBs). Breakthrough technologies in the conversion of solar energy have been identified. A diversification has occurred into globally oriented large power plants producing base load energy, and small scale local on-demand energy supply solutions, also suited for locations without good infrastructure. Decentralised and miniaturised small-scale energy production based on fuel cells provides off-grid energy even in remote areas.

The sectoral relations are expected to change significantly. These structural changes in energy are depicted in picture I.4.



Picture I.4: Expected structural changes in energy supply

Overview of high-priority goals

The high-priority goals as defined in the “Vision & Goals” workshop, besides the general themes as described above, are:

- a. **High-priority goal 1: Increased Renewable Energy Production to 50% of total:** This highly ambitious goal is based on an expected increase in world-wide energy demand by a factor of two in combination with the desire to reduce greenhouse gas emissions to 1990 standards. Increase of conventional, fossil fuel based energy production is not considered a challenge for this sector of the technology roadmap. Shifts in consumption of the various fossil fuel energy carriers, e.g. increased use of natural gas to reduce CO₂ emissions, are also outside the scope of the TRM-Catalysis. On the other hand, conversion of natural gas to liquid hydrocarbons is clearly an area where catalysis plays an important role.

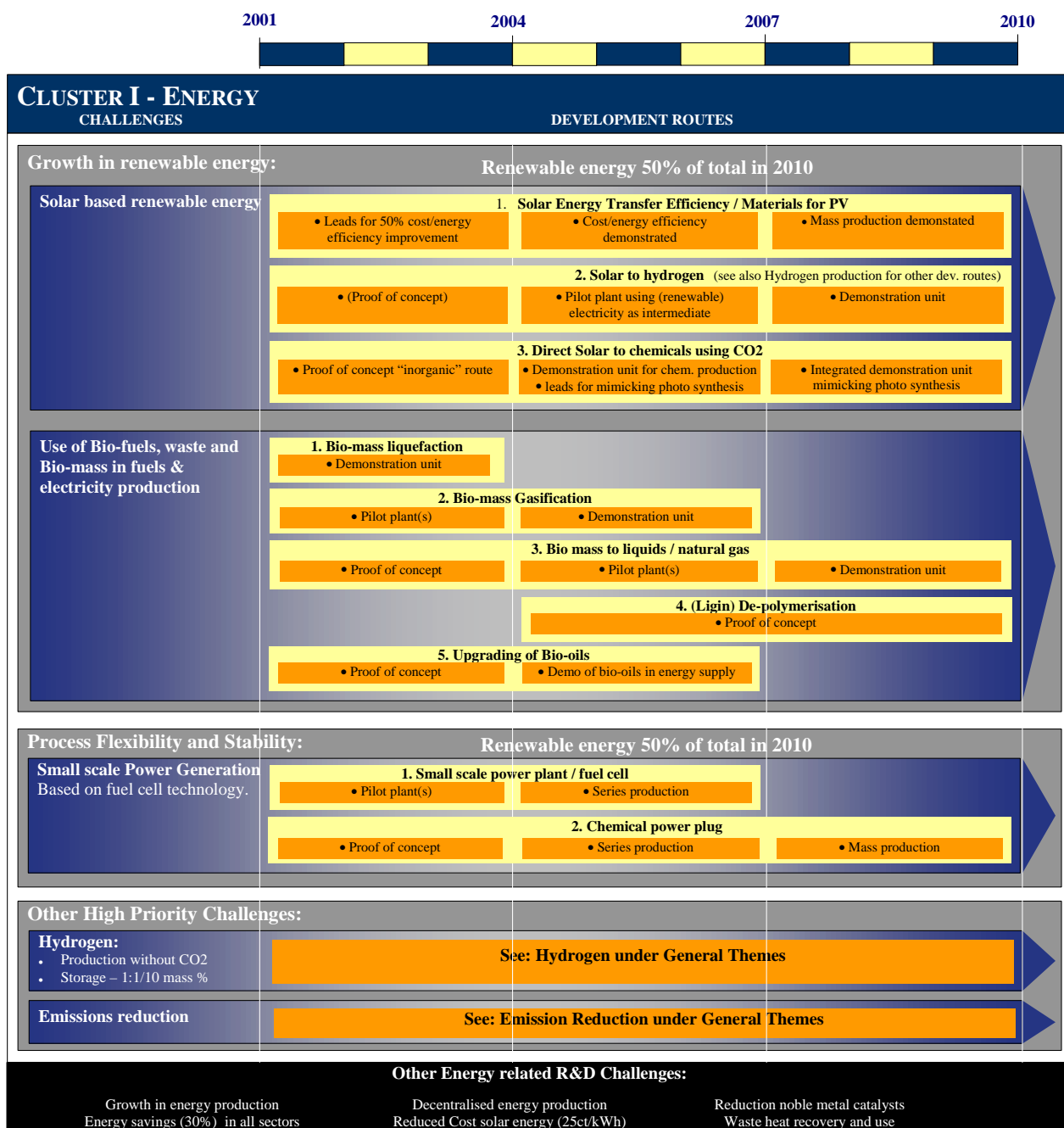
The issues deal with the use of fossil fuels (e.g. noxious emissions and greenhouse gases) are dealt with elsewhere. Therefore, the main challenge is to increase energy production from renewable energy sources; i.e. solar or indirect solar (biomass, wind, hydro). The total amount of bio-mass produced is around 5 Gton per year, or about 50% of crude oil production which is an ample source of renewable energy carrier. It is difficult to specify goals in relation to short-term and long-term, especially since the political debate that should be a driver for the technology development has not been settled yet. In all options, transport, distribution, and storage needs to be considered, as energy production (location and time) is often different from final utilisation.

- b. **High-priority goal 2: Process flexibility and stability:** The end of upscaling in energy production seems to have been reached. Currently, there is a trend to smaller, more flexible units for localised energy production, greatly reducing transmission losses as is already the case for heat (which is produced locally). In addition, smaller units are better capable to adjust energy

production to fluctuations in energy demand with respect to time (peak hours) and location (off-grid). These units range in size from block heating and generating plants to “chemical power plug”; fuel cell based, for miniaturised mobile power supply. The use of renewable energy sources like wind and solar also requires smaller scale power conversion units.

Development Routes

Picture I.5 provides an overview of the additional (in addition to the general themes as previously described) development routes in the Energy sector.



Picture 1.5: Catalysis in Energy Roadmap

High-priority goal 1: Growth in renewable energy production to 50% of total

Contribution of catalysis towards this high-level goal is probably limited to enabling technology and even then to a small extent of the overall goal. Main development routes are:

- a. **Solar Energy:** Considered are direct conversion to electricity (PV), hydrogen production and photosynthesis.

In time the relevant developments are:

- **Short Term : Development of materials for PV** (here a specific link with the polymers sector from Cluster II is obvious); materials with specific properties related to stability to light; organic materials. Photon-electron yield and efficiency improvement with respect to materials manufacturing development (Nano-technology vs. semiconductor industry); fundamental knowledge on the principles of energy transfer in solids using solar energy; silicon chemistry and PV cell design.
 - **Long Term: Direct conversion of solar energy** in the reduction of water to hydrogen or carbon dioxide and water to e.g. methanol; specifically aiming for increased rates of conversion using a wider range of wavelengths of the available light sources (It is important to notice that a significant effort is made for these developments in Japan). Another challenge is the direct conversion of carbon dioxide to e.g. sugars with photocatalysis; mimicking of photosynthetic systems.
- b. **Use of bio-fuels, waste (animal & domestic waste, plastic, “slib”), bio-mass in fuels & electricity production:** Development Options are (super critical) gasification, fermentation, production of ethanol, bio-mass to liquids, synthesis gas conversion technology, selective hydrogenation, supercritical oxidation and selective de-polymerisation (of plastics). In general, catalysis will be an enabling technology in these conversion processes: critical issues are considered in other, (bio-)technological areas. Major driving force is improved efficiency and selectivity of existing technologies especially at lower process temperatures.

In time developments are:

- **Short Term :**
 - **Bio-mass liquefaction (hydrothermal, pyrolysis) and gasification (of bio-mass residue).** New conversion routes for bio-mass, other than complete oxidation (combustion), are currently being investigated up to pilot plant and demonstration units. Main challenges are related to process design and engineering aspects and are outside the scope of catalysis (gasification and hydrothermal liquefaction are basically non-catalytic processes). The specific role for catalysis is in the clean-up of (hot) synthesis gas in that bio-mass will produce different types and levels of impurities which need to be removed before the bio-syngas is used to drive turbines or to produce hydrocarbon gases and/or liquids, or in the clean-up of bio-liquids.
 - **(Bio) SynGas-to-liquids.** Production of transportation fuels from syngas requires high efficiency to C5+ products. The scale of such a process based on bio-syngas is expected to be relatively small in view of feed stock availability, which makes process efficiency even more relevant because of lack of economy of scale.

- **(Bio) SynGas-to-natural gas or fermentation routes to produce methane.** Bio syngas requires special purification treatments before it can be converted to methane. Although methanation itself has been extensively studied, process still needs to be demonstrated and might require specific challenges for catalysis related to the syngas composition. Fermentation is basically a bio-catalytic process; next to methane, ethanol produced by fermentation can be used as energy carrier. These processes can make use of existing distribution networks in e.g. Western Europe but might also help in providing high quality energy carriers in developing countries.
- **Long Term:**
 - **De-polymerisation of plastic waste or bio mass** (lignin) can produce suitable energy carriers (gases and liquids) but also building blocks for the chemical industry.
 - **Bio-technologies** (catalysis and process technology) **for upgrading bio-oils** to make these liquids suitable as transportation fuels.

For all process options discussed a general development is the continuous integration of catalysis and reactor technology. Besides, all process options require more or less an integrated approach of the various technologies listed.

The technological needs in the development routes listed above can be translated to R&D areas as listed below.

Technologies in “Growth of Renewable Energy Production”		
Solar Energy		
1. Solar energy transfer efficiency, solar PV materials.	2. Direct solar to H ₂	3. Direct solar to chemicals / fuels by CO ₂ reduction
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - Photon electron energy yield (basic understanding and materials synthesis) - Polymer materials (organic synthesis and rapid screening) 	<ul style="list-style-type: none"> - Reduced O₂ over-potential (electro-chemistry and material synthesis) 	<ul style="list-style-type: none"> - Photon-electron yield improvement (materials for broader wavelength energy transfer, integration energy transfer materials with (metal) catalysts) - Mimicking photo synthesis (bio-catalysis)
Catalyst Production		
<ul style="list-style-type: none"> - Reduced manufacturing costs 	<ul style="list-style-type: none"> - Increased current densities 	
Process Design		
<ul style="list-style-type: none"> - High surface to volume 		
Process engineering		
Process Monitoring & Control		

Table I.5: Technological focus of catalysis in growth of renewable energy production – Solar based

Technologies in “Growth of Renewable Energy Production”				
Use of bio-fuels, waste, bio-mass in fuels & electricity production				
1. Cracking / gasification / liquefaction / fermentation	2. (Bio) syngas to liquids	3. Bio syngas to ethane	4. Depolymerisation (lignin)	5. Upgrading of bio-oils
Catalyst Design & Discovery				
- Basically non catalytic routes	- Hot syngas purification (catalysts for H ₂ S concentration and C5+ selectivity for liquids)	- Generic catalyst system for variable feeds (waste)	- Modification of existing catalysts (selectivity oxygen removal and stability waste feed impurities)	
Catalyst Production				
- Novel catalyst production routes (layered catalysts)				
Process Design				
- Optimisation of process conditions	- Integration of catalyst with heat transfer			
Process engineering				
- Reactor design				
Process Monitoring & Control				

Table I.6: Technological focus of catalysis in growth of renewable energy production – Bio-based

- c. **Geothermal, wind and hydro based renewable energy sources:** are of great interest but no clear role for catalysis can be identified: at present these energy sources are converted to electricity and power; conversion to hydrogen using electricity as intermediate is described under hydrogen production.

High-priority goal 2: Process flexibility and stability

There is a trend towards combined heat (cold) & electricity production on a local level in (very) small units. These small units facilitate a rapid adjustment of energy production to local and peak demands in that they generally have a much higher turn-up and turn-down rate than typically large scale power plants. The size will vary from block heating and small generating plants to domestic power generation or mobile applications (fuel cell car) to “personal” power generating units for a single device acting as a chemical power plug. These small units require a quick response time (i.e. very active catalysts and therefore low mass), robustness of catalysts and processes to convert a base fuel almost instantaneously to electricity using a fuel cell processor. Miniaturisation of typically large scale conversion units and integration of the various process steps as well as mass-production are new challenges for the catalysis and process technology.

Main technological needs related to these development routes for improved process flexibility and stability are:

- **Fundamental knowledge on concepts**; catalysis tool box for very active and stable catalysts, low mass.
- **Disciplinary Integration** like reactor technology and catalysts
- **ICT as enabling technology** in process control

Technologies in “Process flexibility and stability”	
1. Small scale power plant / fuel cell	2. Chemical power plug
Catalyst Design & Discovery	
- Fast response catalysts (low mass/high activity and high temperature stability)	- Miniaturisation
Catalyst Production	
- Series production	- Series production
Process Design	
- Integration of various catalytic processes	- Integration of various catalytic processes
Process engineering	
Process Monitoring & Control	
- High turn-up/turn down rates	- High turn-up/turn down rates

Table I.7: Technological focus of catalysis in process flexibility and stability

Roadmap Refining

Sector Definition and Vision

Sector definition:

Production of fuels and feed for petrochemical processes by refining hydrocarbon feed-stocks obtained from fossil fuels like crude oil, or synthesised from gas, coal, or methanol.

Description of the sector in 2010:

The future of this sector is strongly related to that of two other sectors, namely transport and energy. It is expected that the oil consumption will increase by 20% in the next decade. The growth will mainly take place in the developing countries. This increase is due to an increasing demand of transport fuels and more specifically due to increasing use of diesel and jet fuels. It is expected that the proportion of diesel-powered transport engines will increase from 15 to 22%, with an expected share of 50% of diesel-powered transport engines in Europe in 2010. The oil usage for power generation and home heating, however, is expected to decrease. In contrast, there is an overall decline in the overall crude oil quality (e.g. 0.2 wt. % more sulphur in oil by 2010). This trend has been announced before, though has not yet materialised. This delay, however, is not in contradiction with the general direction. Thus, chemical technology for a cleaner and more efficient/versatile use of oil products and other feed-stocks will be necessary. For example, taking into account the growing importance of diesel fuels there is a need for more diesel desulphurisation capability in order to meet the new European clean-fuels legislation. Clean fuel components synthesised from existing refinery intermediates (olefins) or future energy carriers like synthesis gas will also be more widely applied. Refinery emissions will be lower. Fuel production for fuel cells may become important for the refiner. New technology for hydrogen production will be required in order to facilitate the need for cleaner fuels. At the same time, the margins on gasoline production will be less interesting for the refiner, so there is a driving force towards petrochemical raw materials (e.g. propylene).

Overview of high-priority goals

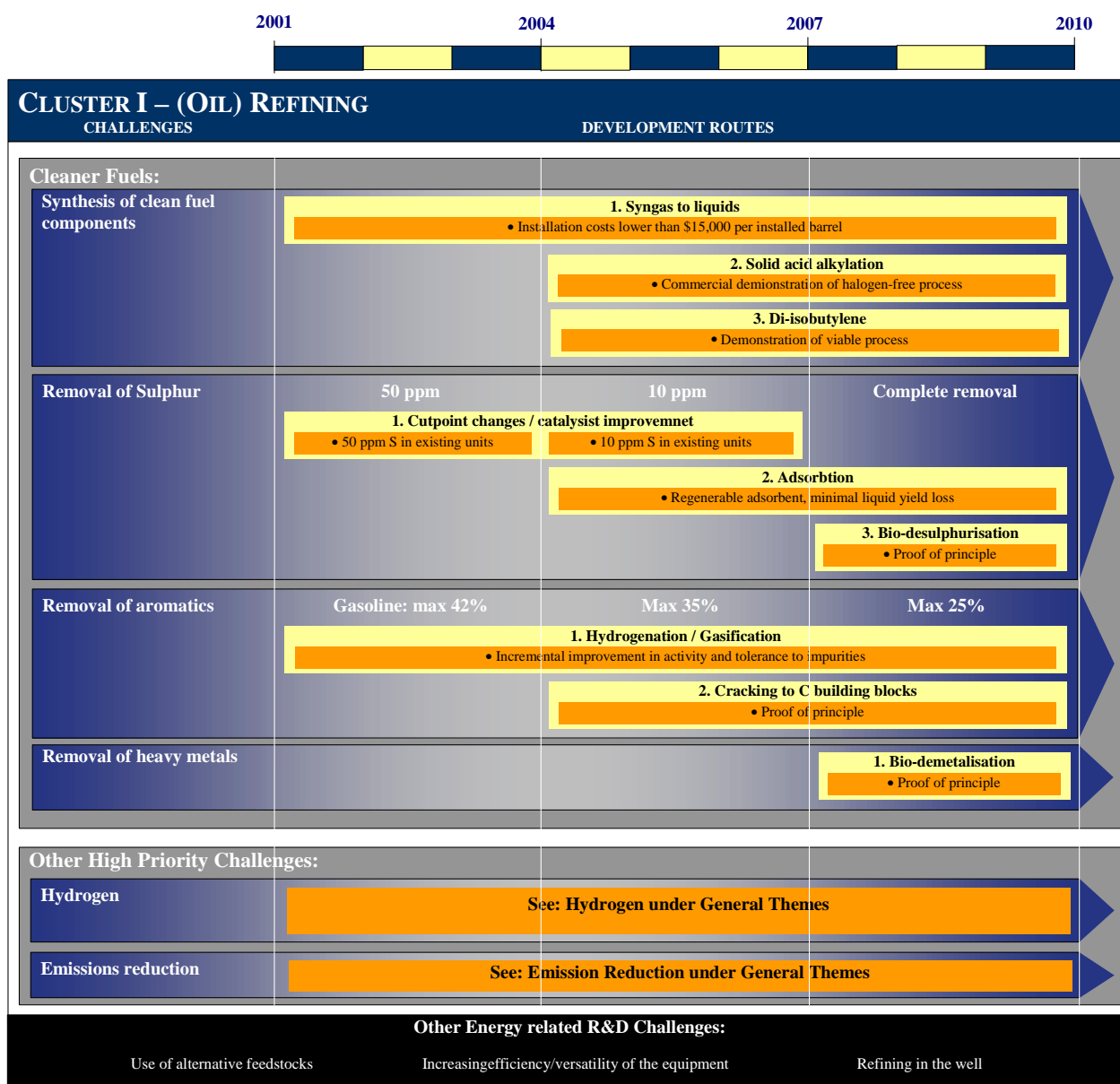
The main goal as defined in the “Vision & Goals” workshop, besides the general themes as described above, is to provide cleaner fuels and feedstocks to the bulk chemicals sector. This strongly relates to the following high-priority goals:

- a. High-priority goal 1: Synthesis of clean fuel components**
- b. High-priority goal 2: Reduction of sulphur - 0 ppm in 2010**
- c. High-priority goal 3: Reduction of aromatics**
- d. High-priority goal 4: Reduction of heavy metals**

In general these goals are related to developments in other sectors of this cluster: if for example, catalytic exhaust gas converters can be made more sulphur tolerant, the need for sulphur reduction in gasoline by refining will become less of an issue. The main driver however, remains legislation. Reduction of nitrogen is not considered a goal: there is merely an enabling technology for refinery conversion processes; current nitrogen content in fuels does not contribute significantly to NO_x. The sector matrices generated after the first workshop list two other high-priority goals: Increasing the production of hydrogen for hydro-processing reactions (HDS, HDN, HDA) and as fuel for fuel power generation, and emission reduction of refineries. These two goals have been shifted from the sector discussion to the overall themes.

Development Routes & Technologies

Picture I.6 below provides an overview of the additional development routes (besides the general themes as previously described) in the (Oil-)Refining sector.



Picture I.6: Catalysis in (Oil-) Refining Roadmap

High-priority goal 1: Synthesis of clean fuel components

In general, removal of undesired components like sulphur and aromatics require hydrogenation processes, which are accompanied by a loss of octane rating, a critical fuel parameter for existing *gasoline* engines. Dedicated synthesis of fuel components with high octane number will become more important. Typically these components are branched paraffin’s, produced by isomerisation of linear paraffin’s or alkylation of small olefins with isobutane; branched olefins like di-isobutylene made by dimerisation; or oxygenates like MTBE. In addition, clean diesel fuels can be manufactured via syngas conversion. The syngas can be produced via gasification of crude oil residuum fractions or from natural gas.

Technological needs are:

Technologies in “Synthesis of clean fuel components”		
1. Syngas to liquids	2. Solid acid alkylation	3. Di-isobutylene
Catalyst Design & Discovery		
	- Solid acids	
Catalyst Production		
- C ₅₊ yield	- Replacement of HF, H ₂ SO ₄	- Relevant
Process Design		
- Relevant	- New process concepts, integral approach (catalyst / reactor)	
Process engineering		
Process Monitoring & Control		

Table I.8: Technological focus of catalysis in synthesis of clean fuel components

High-priority goal 2: Reduction of Sulphur

Reduction of Sulphur is part of the ongoing R&D effort in which catalysis plays a dominant role, especially in the area of fundamental knowledge on the reaction mechanisms. Increased knowledge might result in new processes and catalytic materials. However, at this stage these options are not clearly identified. Integration of catalysts and reactor technology is also part of an ongoing effort in this area. The development is partly driven by legislation. Current EU guidelines indicate an upper limit of 350 ppm sulphur in diesel; in 2005 this will be lowered to 50 ppm. However, most oil companies in The Netherlands started selling 50 ppm diesel in 2001. For gasoline, the specifications are 150 ppm at the moment, and 50 ppm in 2005 (see table I.9 below).

Sulphur content	Up to 1999	2000	2005	2011 ⁽²⁾
Gasoline	500 ppm	150 ppm	50 ppm	10 ppm
Diesel	500 ppm	350 ppm	50 ppm	

Table I.9: Anticipated fuel specifications under the EU Auto Oil Programme II (From Hydrocarbon Processing, September 2000)

Goal related development routes for reduction of sulphur in time are:

- a. **Short Term : Shift of sulphur to (higher) boiling fractions;** *i.e.* from gasoline to diesel and from diesel to residue (bitumen) (“undercutting”).
- b. **Mid Term : Sulphur adsorption** especially to clean up the final fraction of sulphur present which is difficult to convert with the existing hydro-desulphurisation technology.
- c. **Long Term : Bio-desulphurisation:** integral development of (bio)catalysts and reactor technology.

Key technological needs relate to basic understanding, integration catalyst-reactor technology, bio-catalysis and new catalytic materials.

Technologies in “Reduction of Sulphur”		
1. Cutpoint changes / improved catalysts	2. Adsorption	3. Bio-desulphurisation
Catalyst Design & Discovery		
- Better understanding structure / activity relations	- Increased capacity, regenerability	- Relevant (whole cells)
Catalyst Production		
- New preparation routes		
Process Design		
- Low sulphur operation in present equipment	- Minimal liquid yield loss	- Relevant (re-design of units required)
Process engineering		
- Catalytic reactors		
Process Monitoring & Control		
- Improved integration		

Table I.10: Technological focus of catalysis in reduction of sulphur

² EC News Release IP/01/681, May, 11, 2001

High-priority goal 3: Reduction of Aromatics

Aromatics are associated with HSE issues and also needs to be addressed by other technologies like “clean-burning-engines”. Removal of aromatics from fuels requires additional outlet for this stream, which has been considered outside this sector. If aromatics are removed alternatives awill be needed, especially for gasoline engines to maintain fuel properties (e.g. octane rating).

Aromatics content	Up to 1999	2000	2005	2008 (expected)
Gasoline (Total)		42 vol. %	35 vol. %	
Gasoline (Benzene)	5 vol. %	1 vol. %	1 vol. % ⁽²⁾	
Diesel (PNA)		11 wt. %	6 wt. %*	1-4 wt. % ⁽²⁾

Table I.11: Anticipated fuel specifications - EU Auto Oil Programme II (Hydrocarbon Processing, Sept.2000)

Goal related development routes in the area of reduction of aromatics are:

- a. **Short Term : Hydrogenation**
- b. **Mid Term : Gasification**
- c. **Long Term : Cracking** in combination with the use of the residuum as building block (next to bitumen: market for building materials is significantly higher (in mass) than refining sector)

Technological needs are: Again, integral approach of catalysis and reactor technology is considered relevant; “catalytic” combustion of aromatics; separation technology; increase fundamental knowledge in conversion options (phenol is not considered a viable approach)

Technologies in “Reduction of aromatics”	
1. Hydrogenation / gasification	2. Cracking to C-building blocks
Catalyst Design & Discovery	
- Improved basic understanding	
Catalyst Production	
- Incremental improvement	
Process Design	
- Hydrogen technology	- Fundamental knowledge in conversion processes
Process engineering	
Process Monitoring & Control	

Table I.12: Technological focus of catalysis in reduction of aromatics

High-priority goal 4: Reduction of heavy metals

It is not clear whether this goal should be incorporated: heavy metals removal from crude is a necessity to meet specs and to enable existing conversion processes. In view of sustainable development, re-using of these metals is desirable. Heavy metals reduction may thus be a boundary condition rather than a goal.

Main option for development is considered to be Bio-routes for de-metallisation. Synergy is expected in relation to cleaning contaminated soil as well as joint developments with the metal industry. Technological needs are mainly related to electro-chemistry and catalyst regeneration.

Technologies in “Reduction of aromatics”	
3. Bio-demetalisation	
Catalyst Design & Discovery	- Relevant bio-specific methods
Catalyst Production	
Process Design	- Relevant (regeneration, metal recovery)
Process engineering	
Process Monitoring & Control	

Table I.13: Technological focus of catalysis in reduction of aromatics

Roadmap Transport

Sector Definition and Vision

Sector definition:

This sector is concerned with the transportation of people and freight, and the design and production of transport vehicles. The latter includes materials choice, motor design in order to optimise fuel demand and improve recyclability. In a (very) short time-frame, proof-of-principle fuel cell cars can be expected on the basis of hydrogen which is conventionally produced. Major developments will be required in technical issues such as peak power, robustness, but also hydrogen storage and infrastructure. On the middle/long-term we will see the on-board conversion of (fossil) fuels to hydrogen. Additionally, reformer technology has to be modified and improved with respect to catalyst robustness, response time and reliability.

Description of the sector in 2010:

In 2010 the vehicles we use will be much more energy efficient, produce less noise and significantly less emissions, and they will be equipped with intelligent guidance and control systems. Gasoline engines will partly be replaced by (clean) diesel engines, which in turn will be succeeded by fuel cell engines, for which a new infrastructure is being implemented. Consequently, cleaner fuels, derived from existing refinery processes as well as synthetic fuel from i.e. syngas will be used in these vehicles. The preferred hydrogen scenario has been identified: hydrogen storage on board, hydrocarbon conversion or methanol conversion. The increased use of polymer, carbide and composite materials in car bodies has led to weight decrease and a further reduction in fuel consumption. Legislative measures have led to a virtually complete recycling of all vehicle parts. Cars, especially in urbanised areas, will be more oriented towards one or two individuals thus compact cars which are totally recyclable will gain market shares. More intensive use of ship transport, combined road-rail transport and freight transport in road trains will ease the load on highways. This is required to cope with the strongly increased volume of transportation. Air transport will also increase considerably, but aeroplanes will have a much higher fuel efficiency and will be much less noisy. Airports will be completely integrated with other forms of transportation and will have fully automated baggage handling systems, in order to minimise transfer time of people and freight.

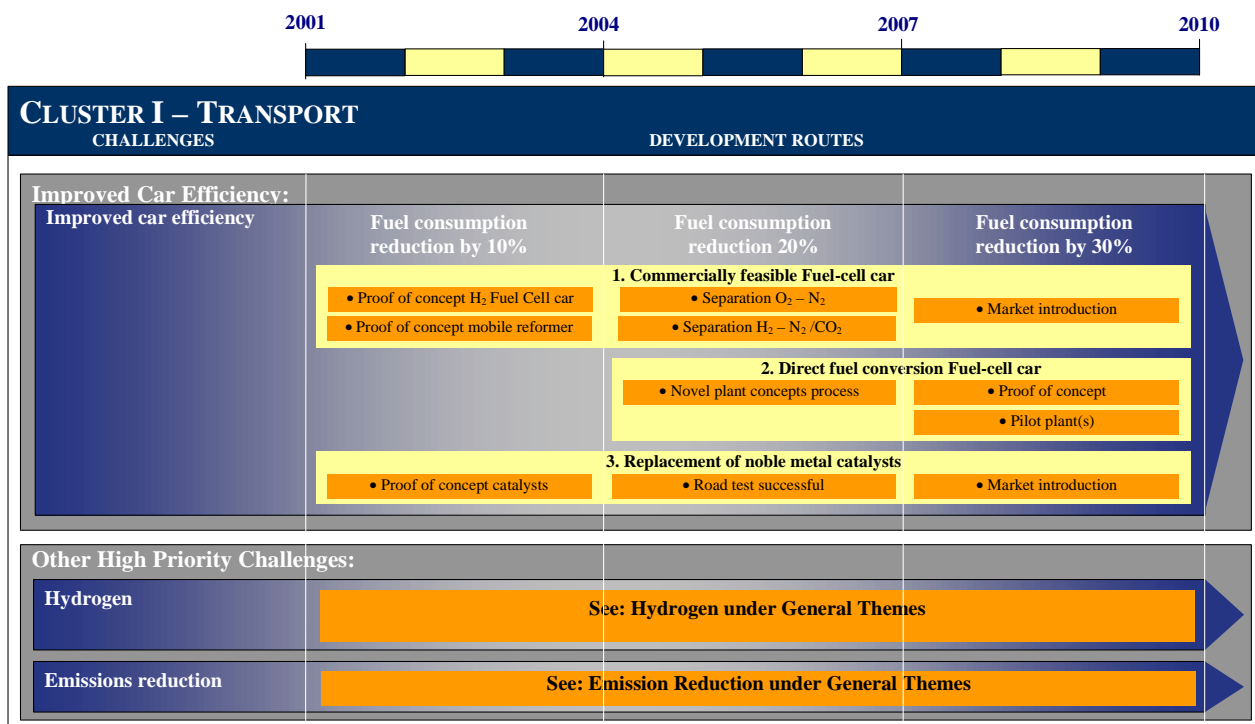
Overview of high-priority goals

The high-priority goals as defined, besides the general themes as described above, are:

- a. **High-priority goal 1: Improved Car Efficiency:** The two main options in reaching this goal are:
- **Lean Burn** (high oxygen / fuel ratio). This option, which is typically valid for diesel cars, gives a higher fuel efficiency. The issue is that catalysts will have to be developed that work under these conditions, as a traditional 3-way catalyst needs richer oxygen-fuel ratios. Therefore, this goal is actually an emission issue, and it is already discussed under the general theme gaseous emissions.
 - **New engine/fuel combinations** (hydrogen, methane, methanol). This is a broad topic, and many parallel routes can be envisaged, but a main theme is the fuel cell car. Fuel cells are clean, fuel-efficient and fuel-flexible. However, there are quite a few hurdles on the way to using them. First, a choice has to be made between the fuels that the car has on board. Either hydrogen can be used directly, or a hydrocarbon fuel is converted on-board in a hydrogen-rich feed gas for the fuel cell. Second, low-cost components are necessary for the system to be competitive, requiring new low-cost, high volume manufacturing methods, and lightweight, compact and affordable hydrogen technologies will have to be developed. Finally, a hydrogen-based infrastructure will have to be realised. These developments will be long-term with legislation as strong push-factor. The goal is a “proof of concept” car which is feasible as new generation vehicle. The type of research required here is highly interdisciplinary.

Development Routes & Technologies

Graph I.7 provides an overview of the development routes (besides the general themes as previously described) in the Transport sector.



Picture I.7: Catalysis in Transport Roadmap

High-priority goal 1: Improved Car Efficiency

Goal related development routes in the area of reduction of aromatics are:

- a. Short Term : Conventional Fuel → Hydrogen → Power** in mobile applications. Specific issues with respect to:
 - Robustness of catalysts, quick response time, reliability, requirements on fuel purity
 - The safety, size and weight of the combined equipment
 - Infrastructure for storage and distribution of hydrogen (this is covered under the general theme hydrogen)
- b. Mid Term: Membrane / separation technology in combination with conversion** (hydrogen enrichment, CO depletion). Combined catalytic functions in membranes.
- c. Long Term (R&D to start on short notice/ongoing, result long term):**
 - Max. 10 ppm CO in hydrogen → two options for development:
 - Reduction using fuel processing technology
 - Increased tolerance of fuel cell
 - Improve fuel cell efficiency – decrease the activation barrier for the electrochemical reduction of oxygen
 - Mobile applications fuel cell – reliability
 - Eliminate use of reformer – direct conversion in fuel cell
 - Replacement for precious metals. A CO tolerant catalyst is also required here.

Technological needs related to these development routes are:

Technologies in “Improved car efficiency”		
1. Commercially feasible Fuel-cell car	2. Direct fuel conversion in Fuel-cell car	3. Replacement of noble metal catalysts
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - Fast response time catalysts, reliability and stability - Catalytic membrane materials 	<ul style="list-style-type: none"> - Robust catalysts - Understanding deactivation mechanism 	<ul style="list-style-type: none"> - High throughput materials screening - Understanding structure / activity relations
Catalyst Production		
<ul style="list-style-type: none"> - Production of high permeability (cat.) membranes 	<ul style="list-style-type: none"> - Improved CO resistance 	<ul style="list-style-type: none"> - New preparation routes
Process Design		
<ul style="list-style-type: none"> - Process integration and modelling 	<ul style="list-style-type: none"> - Process integration and modelling 	
Process engineering		
<ul style="list-style-type: none"> - Analysis hardware - Miniaturisation 		
Process Monitoring & Control		
<ul style="list-style-type: none"> - Fast response process monitoring 	<ul style="list-style-type: none"> - Fast response process monitoring 	

Table I.14: Technological focus of catalysis in improved car efficiency

4. CLUSTER II: BULK CHEMICALS, POLYMERS & MATERIALS AND DETERGENTS & TEXTILES

Introduction to Cluster II

Cluster II consists of the sectors Bulk Chemicals, Polymers & Materials and Detergents & Textiles. Cluster II encompasses a wide variety of products and production volumes: from a bulk chemical like ethene, which is produced world-wide in over 50 10⁶ ton/year and for which price is the main differentiating factor, to special polymers for electronic applications, which are currently produced on < 1 ton scale and where performance is the differentiation. Similarly, required catalysts range widely from, for example, expensive ones for use in single batch to cheap and robust catalysts for use in large-scale continuous processes or from homogenous to supported homogenous to truly heterogeneous catalysts.

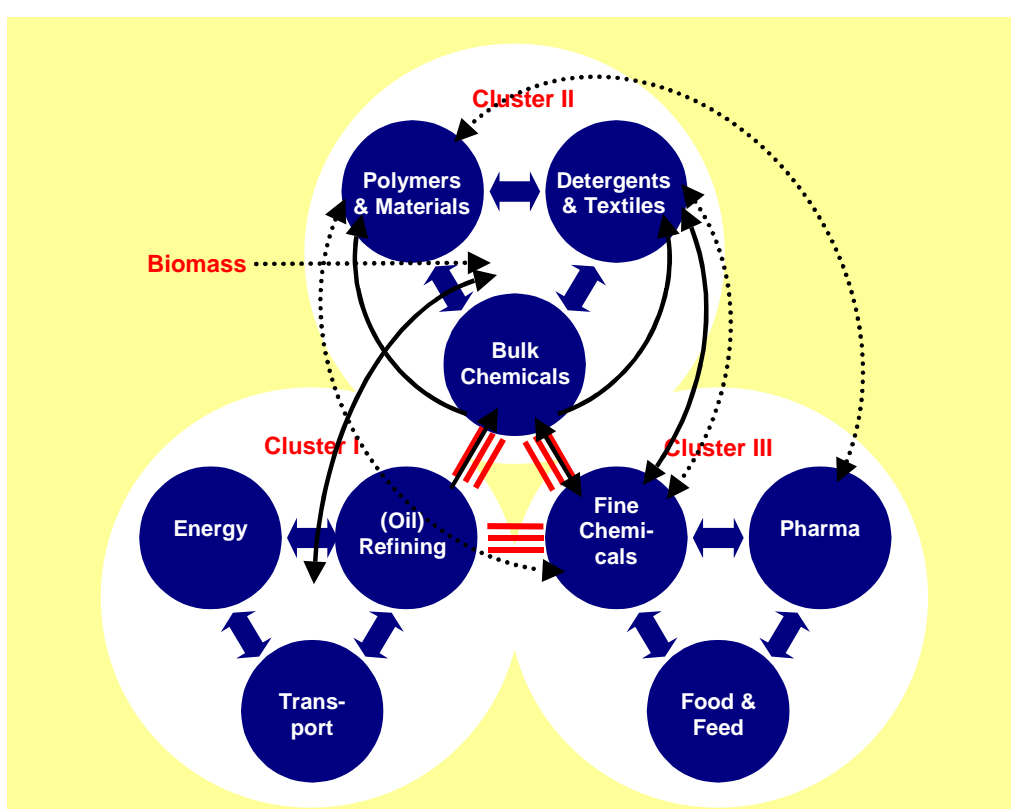
The increasing acceptance of the concept of sustainable development and cluster II's almost exclusive reliance on feedstocks produced by the Energy, Refining and Transport cluster offer exciting challenges:

- a. Cluster II is very dependent on finite fossil resources, in particular oil, to provide:
 - the carbon atoms, which are key building blocks of its organic products
 - the energy to drive its processesDepletion of finite fossil resources and/or emission of CO₂ are not compatible with sustainable development.
- b. Cluster II has come to be very reliant on the Energy, Refining and Transport cluster as source of its prime feedstocks like ethene, propene, aromatics, and synthesis gas. Boldly put, however, these feedstocks are only side-products of the fuel production of cluster I (through cracking of crude oil), which is considered to be the more important activity of cluster I. As less than 10% of the fossil feedstocks end up as (petro)chemicals, it is evident that Cluster II is highly dependent on developments initiated and products produced by the dominant user of fossil resources, cluster I. If, for example, cluster I moves away from crude oil as feedstock to hydrogen as prime source of energy and mobility, ethene and propene will no longer be produced as cracker side-products by cluster I. Cluster II will therefore be faced with a shortage of starting materials it has come to rely on. Similarly, if natural gas, coal or biomass replace crude oil as feedstock for fuels cluster II may have to revert to the use of e.g. synthesis gas, alkanes, methanol or ethanol as prime feedstocks. Thus, in the end, the currently highly intertwined sectors I and II may become completely decoupled.
- c. Biomass and/or recycled products as feedstock – a variety of schemes have been devised to reduce dependency on fossil feedstock in order to comply with principles of sustainable development. However, universally accepted metrics to assess attractiveness of these options are not available yet.

In the past the cluster could be rightfully called a truly Dutch cluster: Dutch companies producing products in The Netherlands from building blocks produced in The Netherlands based on research conducted in The Netherlands. With the ongoing globalisation this is no longer true. Hence, realisation of the longer-term goals for this cluster cannot come from isolated Dutch initiatives.

Relations between sectors

The current relations within cluster II are currently clearly one-way: Bulk Chemicals being the feedstock supplier to the Polymers & Materials and the Detergents & Textiles sector (see figure below). In the future, when recycling of products becomes more prominent, a two-way situation will emerge from the Polymers & Materials and possibly the Detergents & Textiles sectors becoming suppliers of feedstock to the Bulk Chemicals sector (closed loop situation; indicated by dashed arrows).



Picture II.2: Relations between sectors as seen from a cluster II perspective. Existing relations and their directions are indicated by arrows, future relations are indicated by dashed arrows.

Relations between clusters II and I currently hinge primarily around Bulk Chemicals with the Refining sector of cluster I currently being a major source of (starting materials for) Bulk Chemicals such as ethene, propene, aromatics, and synthesis gas ($\text{CO} + \text{H}_2$). As discussed in description of sector II and in the development routes for cluster I, the future relations between clusters II and I may change as cluster I moves towards energy production from renewable resources and hydrogen. In one scenario the remaining oil will then be used as feedstock for chemicals in a similar fashion as today (i.e. a more sustainable use of this carbon source than combustion to CO_2). Alternatively, the development of alternative feedstocks for cluster I might result in other starting materials becoming abundantly and cheaply available as feedstocks for

cluster II. Examples are synthesis gas (mixture of H₂ and CO - obtained from natural gas, coal or biomass, and as such could serve as a feedstock-independent “*linga franca*” for the petrochemicals industry), alkanes (from natural gas), ethanol (from biomass), or lignin (remaining as waste after fermentation of biomass to e.g. ethanol). In yet another scenario, clusters I and II become completely decoupled with sector II now taking care of its own feedstock situation through for example the dedicated production and processing of biomass. In all likelihood, a mixture of the aforementioned scenarios will play out in the next 25 years.

The Bulk Chemicals sector is a major supplier of starting materials, reagents, and solvents to the Fine Chemicals sector of cluster III and thus indirectly also to the Pharma and Food & Feed sectors. Interaction of the Polymers & Materials sector with cluster III (Fine Chemicals, Pharma and Food & Feed sectors) will continue to increase: next to the current use of polymers for packaging, applications like special polymers for slow release of medicines or selective membranes for purification purposes will become significant. Vice versa, the relation with Fine Chemicals in Sector III as source for catalysts and monomers for speciality polymers will increase. An additional link exists between the bleach catalysts used in the Detergents & Textiles sector of Cluster II and the Fine Chemicals sector (Cluster III), which employs the same catalysts for non-aqueous oxidation reactions.

Roadmap Bulk Chemicals

Sector Definition and Vision

Sector definition

The Bulk Chemical sector is defined as Synthesis of Bulk Chemicals with a production of more than 10,000 ton per year. (per single production unit).

Sector in 2010

In 2010 the chemical industry will produce bulk chemicals at virtually 100% selectivity and consequently with very little environmental impact. The processes will be highly energy efficient and the use of alternative and renewable feedstocks either directly or indirectly will be economically attractive. For many purposes the composition of these feeds is largely flexible as they will be converted mainly into synthesis gas (CO+H₂), which in turn will become the building block for further synthesis (methanol / Fischer-Tropsch). In some cases these feedstocks will be subject to a pre-treatment procedure, e.g. in the case 'heavier' (oil-based) feedstocks are used. In other cases, bio-feedstocks will be used directly for chemical synthesis (e.g. ethanol, lactic acid, etc.). In addition, a shift will take place in the use of alkanes rather than olefins for the production of (more complex) chemicals. The overall downtime of plants will have decreased due to the use of improved materials, better process control and increased stability of catalysts. The production facilities will be locally concentrated, highly integrated, and considerably smaller in size. The manpower associated with bulk chemicals production will be almost nil.

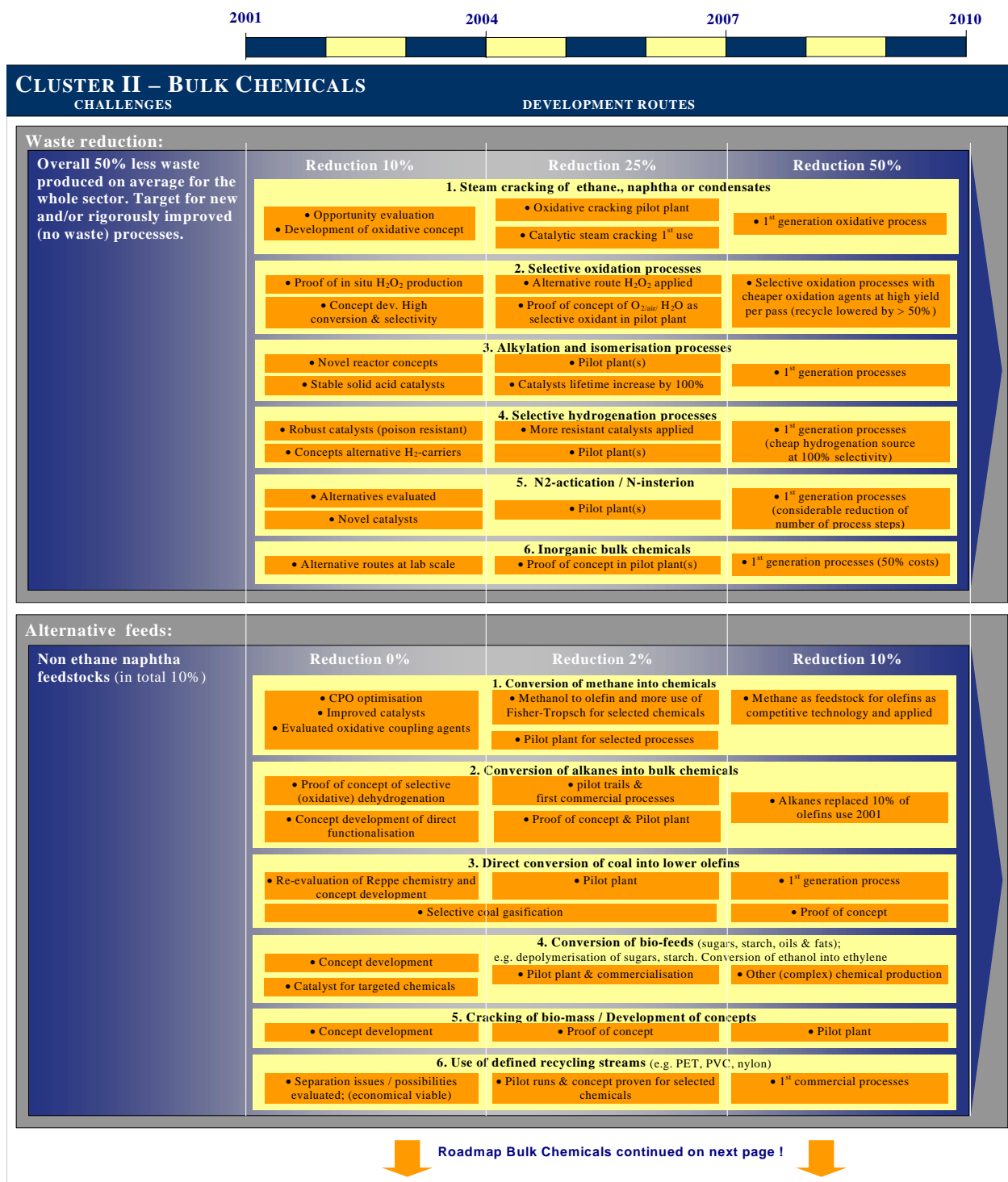
Overview of high-priority goals

The high-priority goals as defined in the “Vision & Goals” workshop in the Bulk Chemical sector are:

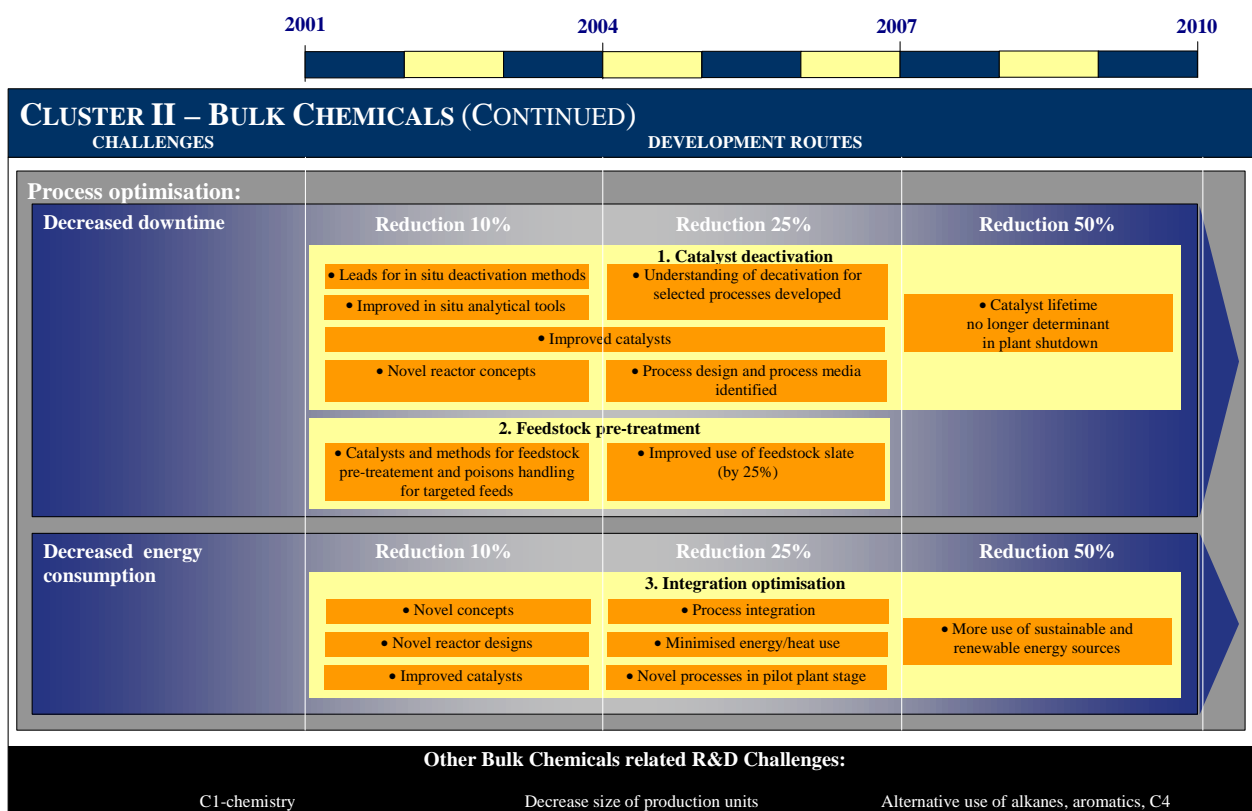
- a. **High-priority goal 1: Waste reduction** – overall 50% less waste produced on average for the whole sector. The target for new and/or rigorously improved processes – no waste (excluding CO₂ / H₂O production). Catalyst waste itself will need to be decreased and catalyst waste treatment procedures will need to be developed.
- b. **High-priority goal 2: Alternative feeds** – 10% of the feedstock not derived from naphtha / ethane
- c. **High-priority goal 3: Process optimisation:** Consisting of:
 - **Decreased downtime** through increased catalyst lifetime and/or decreasing production of by-products at end of run conditions – downtime decrease by 50%
 - **Highly integrated and energy efficient production facilities** – decrease energy consumption by 50%

Development routes

Pictures II.3 and II.4 below provide an overview of the development routes in the Bulk Chemicals sector.



Picture II.3: Catalysis in Bulk Chemicals Roadmap



Picture II.4: Catalysis in Bulk Chemicals Roadmap (continued)

High-priority goal 1: Waste reduction

Waste reduction is considered a high-priority goal because manufacture of non-desired products is an inefficient use of feedstocks and energy. In addition, government legislation, public opinion and costs associated with waste disposal are strong drivers. More selective catalysts and processes will play an important role in minimising waste. Exergy analysis of both existing and new processes will continue to be important and lead to more energy efficient processes.

Processes with a large potential impact on this goal are:

- a. **Steam cracking of ethane, naphtha or condensates:** Presently cracker feedstock depends heavily on the local situation, i.e. on the availability of certain feeds and resident markets. Crackers are often built where certain feeds are readily available, priced favourably, integrated into an ethylene pipeline, etc. A clear desire is to be able to more selectively crack a broad variety of feedstocks, ranging from the traditional ones used today to bio-feeds, recycled products, etc. Presently steam cracking is non-catalytic and the product composition depends largely on the feedstock used. It is highly desirable to be able to tune and control the product slate, e.g. ethylene/propylene ratio. The capital investment for crackers is huge and needs to be decreased. Other potential processes than traditional steam cracking are desired (e.g. oxidative catalytic routes).

Catalyst development, reactor and process design are important issues. It will be necessary to develop novel catalysts that can control the desired product slate. Rapid screening techniques can be applied to build up a database for catalyst design. Controlling the heat of reaction in the oxidative route through reactor design (e.g. fluidised bed) is important as is the envisaged integration into the downstream distillation. Obtaining knowledge on the kinetics is essential. Key technological issues are:

- Catalytic steam cracking. Developing stable catalysts that can control / influence the product ratio / composition.
- Oxidative cracking. Exothermic and selective cracking using O₂ or air. Reactors with very short residence times (e.g. Lanny Schmidt set up). Selective and novel catalysts are required.

- b. Selective oxidation processes:** Many processes now run at low conversions per pass and / or use expensive oxidation agents like e.g. H₂O₂. Low conversions are often required to prevent ‘over’ oxidation or run-away reactions (e.g. to CO₂). Oxidation reactions are often very exothermic and controlling the heat of reaction is important. Hot spots can give rise to non-selective reactions further enhancing heat release. Low conversion processes are generally energy costly due to the product separation steps involved. Thus high conversion routes using cheap(er) oxidants such as air, oxygen or CO₂ are very attractive.

Oxidation reactions are typically very exothermic. Therefore to obtain high conversions per pass while maintaining a high selectivity is a challenge. Reactor and process design are especially important besides catalyst development. Breakthrough approaches are needed to be able to use cheap oxidation agents such as air and water selectively. Key issues technological are:

- Achieve high selectivity at high conversions leading to less recycle and a more (energy) efficient processes
- Integration of catalyst and reactor concept (membranes / reactive distillation)
- Synthesis of hydroperoxides or H₂O₂ in situ, e.g. through controlled addition of H₂ and O₂
- The use of water, air or oxygen as selective oxidant
- Direct route for benzene to phenol (oxidation by water)

- c. Alkylation and isomerisation processes:** Many processes presently use strong acids and traditional Friedel-Crafts catalysts like HF, H₂SO₄, AlCl₃, etc. These catalysts often need to be separated from the product and then neutralised. Typically the energy used and the waste generated for cleaning and / or disposing of these acid waste streams is considerable. Besides, thermodynamic equilibria often exists requiring (large) recycle streams. More selective, direct catalytic routes generating less waste are desired; i.e. alternatives are needed for the typical Brønsted and Lewis acid catalysts.

A problem of potentially interesting processes is the rapid deactivation of the catalyst. Special emphasis on reactor design and novel process approaches is therefore valuable. Determining the kinetics of the reaction and deactivation will provide helpful data. Key technological issues are:

- The development of stable, regenerable solid acids, e.g. zeolites (alkane and aromatic alkylations)
- Novel reactor concepts (rapid catalyst recycle, fluid bed, etc.)
- Avoiding thermodynamic limitations (membranes, reactive distillation, etc.)

- d. Selective hydrogenation processes:** Several processes require selective hydrogenation steps. A high selectivity is desired either to save feedstock cost, lower separation costs, or limit undesired reactions of the product in a subsequent reaction step. Examples are benzene to cyclohexene (for caprolactam), phenylacetylene to styrene and acetylene to ethene.
- Many selective hydrogenation processes exist today. Still improvements can be made in the overall effectiveness of these processes. Key technological issues are:
- The development of more selective catalysts
 - Alternative (cheaper) reduction agents / H₂-carriers
 - More resistant catalysts (e.g. the use of less pure H₂ containing CO)
- e. N₂-activation / N-insertion:** Insertion of N-atoms into a hydrocarbon is presently cumbersome and often involves several steps, e.g. acrylonitrile, caprolactam, amines, aniline, etc. For instance, all commercial caprolactam processes produce ammonium sulfate as a by-product. It either originates from the use of sulfuric acid to convert cyclohexanone oxime to caprolactam and/or from the production of hydroxylamine to manufacture cyclohexanone oxime. Ammonium sulphate is even produced in excess of the amount of caprolactam and is sold as a (low value) fertiliser. It is clear that it would be advantageous if more economical, direct route could be developed. This also holds for many of the other nitrogen-containing chemicals mentioned above.
- Breakthrough approaches are required in several instances. Nitrogen insertion and activation is difficult and often requires several process steps. Combination of several steps into one is challenging. Catalyst development in combination with novel reactor concepts, e.g. the use of a riser reactor, is an important feature. Key technological issues are:
- Development of concept
 - Novel catalysts
- f. Inorganic bulk chemicals:** Alternative, more selective routes to bulk chemicals such as H₂SO₄, H₃PO₄, NH₃, urea and ammoniumnitrate are attractive. For instance, for the oxidation of SO₂ to SO₃ vanadium containing solid (catalyst) waste is produced and the conversion efficiency is not 100% (typically 98.5%). Even more solid waste is generated if other sources than elemental sulphur are used as starting material. It would be advantageous if a cleaner and more efficient process could be developed. A direct production route of sulphuric acid from SO₂ could also be attractive.
- Further improvements in the (commercial) ammonia catalysts are also possible. Both the alkali-promoted Fe- and the Ru/C-catalysts can be improved, e.g. an alternative support for Ru is desired because gasification of carbon takes place under reaction conditions. Also the dispersion of the (expensive) Ru can be improved. A novel route and/or process and reactor design should also be taken into account.
- The technologies needed depend on the specific process. Key technological issues are:
- Development of novel more robust catalysts
 - Novel process

The table underneath provides an overview of technological needs for each of the development routes for waste reduction as described above.

Technologies in “Waste Reduction”		
1. Alternative steam cracking	2. Selective oxidation	3. Alkylation / isomerisation
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - High selectivity catalyst discovery - High throughput (database) 	<ul style="list-style-type: none"> - High yield catalyst (selectivity at high conversions) 	<ul style="list-style-type: none"> - Catalyst optimisation (deactivation)
Catalyst Production		
Process Design		
<ul style="list-style-type: none"> - Heat generation control - Reactor concept (O2 introduction) 	<ul style="list-style-type: none"> - Integration of catalyst - Use of air - Reaction kinetics 	<ul style="list-style-type: none"> - Integration of catalyst - New process media
Process engineering		
<ul style="list-style-type: none"> - Integration of heat - Kinetics 	<ul style="list-style-type: none"> - Kinetics 	
Process Monitoring & Control		
<ul style="list-style-type: none"> - In situ analysis 		

Table II.1: Technological focus of catalysis in waste reduction

Technologies in “Waste Reduction” (Continued)		
4. Selective hydrogenation	5. N₂ activation / insertion	6. Inorganic bulk chemicals
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - Catalyst optimisation (selectivity) 	<ul style="list-style-type: none"> - Catalyst discovery 	<ul style="list-style-type: none"> - Catalyst optimisation - Catalyst discovery
Catalyst Production		
Process Design		
<ul style="list-style-type: none"> - Method of H2 addition / H2 carriers 	<ul style="list-style-type: none"> - Reactor concept 	
Process engineering		
Process Monitoring & Control		
<ul style="list-style-type: none"> - In situ rapid analysis 		

Table II.1(continued): Technological focus of catalysis in waste reduction

High-priority goal 2: Alternative feeds – 10% of the feedstock not derived from naphtha / ethane

Processes with a large potential impact on this goal are:

- a. Conversion of methane into bulk chemicals either via synthesis gas or methanol:** It would be attractive to be able to convert methane into liquid fuels or chemicals. It is often commercially unfeasible to transport methane from e.g. remote oil fields to desired locations for consumption as fuel. The result is that large amounts of methane are being flared. Estimations have been that e.g. the amount of methane produced with crude oil and subsequently flared for disposal is equivalent to 1 million barrels of oil per day. In other cases, recoverable natural gas resources lie in remote locations or in smaller accumulations that make economical exploration unattractive due to high transportation costs. Attractive methods of capturing the value of this methane could be converting into (bulk) chemicals through initial conversion into either synthesis gas or methanol. Synthesis gas can subsequently be converted by e.g. Fischer Tropsch into chemicals as can be methanol by alternative methods. Methanol is also more easily transportable than natural gas. The growing trend to use feedstocks of various sources and the emphasis on sustainable chemistry can put a strong push on the use of synthesis gas as a more generic feedstock.

Much research has already been put and is still being put in this area. Further improvements are needed in catalyst optimisation (selectivity and stability). Developing novel reactor concepts to avoid over oxidation and control the heat of reaction (for the oxidative case) are also important. The current problems are the inclusion of several process steps and the large capital requirement. Improvements can be expected from the improvement of the individual steps and the elimination of steps. A solution could be interwoven with other technologies, e.g. the N_2/O_2 separation of air.

Other technological needs are:

- Further catalyst development
 - Optimisation of catalytic partial oxidation (CPO), improving catalyst stability and resistance to poisons
 - Development of inorganic membrane reactors
 - Controlled Fischer-Tropsch (chain length and functionalisation)
 - Direct methanol synthesis routes
 - Methane to olefins (oxidative coupling)
- b. Conversion of alkanes into bulk chemicals:** In the early 1900s, many bulk organic chemicals were derived from acetylene rather than ethylene. After petroleum became a major feedstock, one of the main building blocks for bulk chemicals became ethylene. Alkanes are attractive starting materials, especially considering their relative pricing versus alkenes. However, alkanes are much more difficult to “activate” for chemical synthesis purposes. Illustratively, ethane is cracked into ethylene in the modern chemical industry. Hence it would be very attractive if direct routes to chemicals from alkanes could be developed, e.g. production of oxygenates, amines, etc. The first developments in this direction are already taking place and it can be expected that the significance of the use of alkanes in the chemical industry will increase.

More or less the same issues are important as is the case with methane activation. These are:

- Selective and stable (oxidative) dehydrogenation catalysts
- Direct functionalisation methods (*e.g.* oxygenation, amination)
- Novel reactor concepts (general purpose reactors)

- c. Direct conversion of coal into lower olefins:** As indicated above, much of the early based chemical industry was based on acetylene chemistry. Butadiene made from acetylene was the basis of synthetic rubber. Acetylene was initially produced by a process using limestone and coal. Calcium carbonate (limestone) was first converted to calcium oxide, and coal was converted to coke. These two products were reacted to produce calcium carbide. Acetylene was then formed from calcium carbide by reaction with water. Acetylene can also be produced directly by the reaction of coal and hydrogen at high temperatures. Since oil reserves are diminishing, acetylene may once again become an attractive raw material for many commercial products. Walter Reppe pioneered the study of acetylene chemistry at high pressures and was able to synthesise many valuable chemicals. Since the introduction of ethylene as basic building block, the practical importance of this chemistry has diminished. A modern re-evaluation of this Reppe chemistry for the production of bulk chemicals is worthwhile in view of the longer-term energy scenario. Re-evaluation of (old) Reppe chemistry is needed. With the present understanding and technology capabilities this chemistry might be attractive, especially based on the assumption that more carbon-rich molecules will be used for chemicals in the future. H₂-rich molecules will be used for fuels.

Other key technological issues are:

- Further development of technologies for the gasification of coal
- Development of catalysts for the use of acetylene as feedstock (rapid screening)

- d. Conversion of bio-feeds** (sugars, starch, oils & fats); *e.g.* depolymerisation of sugars, starch. Conversion of ethanol into ethylene: The world's oil reserves are depleting at a steady pace. Cost effective petroleum alternatives derived from renewable resources such as corn, sugars and starch will become more important. A present development is the selective removal of cellulose from corn fibre and the isolation of the xylose and arabinose fractions. These can then be catalytically converted into *e.g.* ethylene and propylene glycol. Conversion routes of cellulose to chemicals are also being looked into. Another example is the use of lactic acid for the production of polylactic acid (PLA). The importance of bio-feeds is expected to increase further. Catalysts will need to be developed to economically convert renewable resources into valuable chemicals.

Key technological issues are:

- Concept development. To be used for the synthesis of targeted chemicals
- Selective and stable catalysts

e. Cracking of biomass / Development of concepts: Biomass can be obtained from numerous sources such as agricultural crops, forests and major parts of household waste. Biomass is increasingly being used for power generation and from a fundamental point of view it should be considered for the production of chemicals. Biomass can be converted at high temperature and high pressure into biocrude, an oil-like substance which can be used for energy purposes or for the synthesis of chemicals. Research areas to focus on are: the production and treatment of biomass feedstocks and the conversion of the feedstocks into (high-value) chemicals. A possible approach could be to convert biomass to synthesis gas, which is then subsequently cleaned and conditioned to produce desired chemicals. Another approach could be biomass pyrolysis. This produces a mixture of oils, char, and non-condensable gases, which can be further processed to derive a variety of products. The oils can be condensed to form a biocrude which, after treatment, can then be used for targeted chemicals production.

Biomass is a generic term for complex biological mixtures with a varying composition depending on the source. When envisaging chemicals production using these sources, general upgrading methods must be looked into. Gasification into basic building blocks (CO and H₂) or conversion into a liquid biocrude are possibilities. Other than this technological issue, concept development and especially the economics must be looked into.

f. Use of defined recycle streams, e.g. PET, PVC, nylon, polyamide: There are several methods to recycle chemicals, one being direct reuse. Although this is a good option in certain cases (e.g. PET for bottles), it is more difficult in others. The focus here involves the use of polymer waste arising from the pyrolytic, chemolytic or (catalytic) hydrocracking processes used to break down polymeric waste into simpler substances, preferably monomers which subsequently can be reused. In some cases this can be done to obtain specific molecules (e.g. styrene), in others non-specific pyrolysis products will be obtained such as methane, ethane, ethylene, propene, benzene, etc. This can then be treated in existing (integrated) production facilities. Technology is also available that can convert unsorted plastic waste into a diesel type oil that, in principle, can be used for the production of chemicals.

Several polymers can be recycled effectively. However, contamination and waste separation issues make this difficult. Attractive novel methods for separation and/or general use of the overall (polymeric) waste stream are attractive options.

Key technological issues are:

- Separation issues. Determine economical separation methods for the various plastics & blends (PVC, PE, etc.). Longer-term issues like preventing the use of blends and / or additives.
- Novel process concepts
- Novel process media

The table below provides an overview of technological needs for waste reduction.

Technologies in “Alternative feeds”		
1. Methane to bulk chemicals	2. Alkanes to bulk chemicals	3. Coal to olefins
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - Catalyst optimisation (stability) - Catalyst (FT / direct methanol) 	<ul style="list-style-type: none"> - Catalyst discovery - High throughput - Direct functionalisation 	<ul style="list-style-type: none"> - Catalyst discovery (screening)
Catalyst Production		
Process Design		
<ul style="list-style-type: none"> - Heat generation control - Reactor concept - Kinetics 	<ul style="list-style-type: none"> - Reactor concept - Reaction kinetics 	<ul style="list-style-type: none"> - Gasification technology - Novel concepts
Process engineering		
<ul style="list-style-type: none"> - Integration of heat 		
Process Monitoring & Control		

Table II.2: Technological focus of catalysis in alternative feeds

Technologies in “Alternative feeds” (Continued)		
4. Conversion of bio-feeds	5. Cracking of bio-mass	6. Defined recycle streams
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - Catalyst discovery (selectivity) 	<ul style="list-style-type: none"> - Catalyst discovery (activity & selectivity) 	<ul style="list-style-type: none"> - Catalyst discovery (selectivity & poison resistance)
Catalyst Production		
Process Design		
<ul style="list-style-type: none"> - Method of H₂ addition / H₂ carriers 	<ul style="list-style-type: none"> - Reactor concept 	<ul style="list-style-type: none"> - Separation issues - Novel process media
Process engineering		
<ul style="list-style-type: none"> - Integration into present production 		
Process Monitoring & Control		
<ul style="list-style-type: none"> - In situ rapid analysis 		

Table II.2 (continued): Technological focus of catalysis in alternative feeds

High-priority goal 3: Process optimisation

The high-priority goal of process optimisation consists of two main elements. These are:

- a. Decreased downtime through increased catalyst lifetime and/or decreasing production of by-products at end of run conditions – downtime decrease by 50%:** The goal related products and processes are very application specific. However, general knowledge on various *deactivation mechanisms* (e.g. *coking, ligand degradation, enzyme denaturation*) remains important. Also *feedstock pre-treatment methodologies* will be important to be able to use wide feedstock slates of varying quality. Improvement of the catalyst stability also remains of vital importance.

The key technological issues in this area are:

- **Catalyst Technologies:** Studies related to obtaining information on the various deactivation methods are important. Analytical in-situ techniques will need to be developed to be able to study catalysts under real working conditions. Other issues are the possible reactivation of catalysts and the development of more robust and poison resistant catalysts (highly process specific).
 - **Process Concepts:** Novel reactor concepts e.g. reactive distillation, fluid and moving beds can be applied in certain instances. In homogeneous systems novel process media (e.g. ionic liquids) or the use of different solvents can be envisaged. Possibly module technology can be applied to cope with rapidly deactivating catalysts (sequential continuous regeneration).
 - **Analysis Applications:** Unravelling of deactivation mechanisms.
- b. Highly integrated and energy efficient production facilities – decrease energy consumption by 50%:** In principle, this is relevant for all bulk chemical processes (direct downstream use, transport of energy). The application of co-generation (integration of electricity & steam production) in chemical production facilities will increase. Novel reactor technology and concepts play an important role in achieving this goal. The development of more active and selective catalysts will also increase the energy efficiency of several processes. In some instances a novel breakthrough approach will lead to significant energy savings, e.g. combination of oxidative coupling of methane process into gas turbine technology. High temperatures are used to (catalytically) burn methane to drive turbines. Similar temperatures are required for the oxidative coupling of methane. A combination of gas turbine technology and the co-production of ethylene might be an attractive option. Further integration of exothermic with endothermic processes is also a possibility. These features will be highly process and site dependent. It might also be possible to more effectively use waste streams (e.g. flares) for heating purposes or for the production of (clean) water (water treatment). Longer term options include the use of sustainable energy sources.

The key technological issues in this area are:

- Process & Reactor Technologies
- Development of catalytic reactor technology; novel concepts

The table below provides an overview of technological needs for each of the development routes for waste reduction as described above.

Technologies in “Process optimisation”		
1. Catalyst deactivation	2. Feedstock pre-treatment	3. Highly integrated and energy efficient production facilities
Catalyst Design & Discovery		
<ul style="list-style-type: none"> - Catalyst optimisation - High throughput (promoters, stabilisers) 	<ul style="list-style-type: none"> - Catalyst optimisation 	<ul style="list-style-type: none"> - Catalyst selectivity (less by-products)
Catalyst Production		
<ul style="list-style-type: none"> - Robust, high quality catalysts 		
Process Design		
<ul style="list-style-type: none"> - Deactivation kinetics - Reactor concept - Process media 	<ul style="list-style-type: none"> - Deactivation kinetics 	<ul style="list-style-type: none"> - Reactor concept
Process engineering		
<ul style="list-style-type: none"> - Integration optimisation 		
Process Monitoring & Control		
<ul style="list-style-type: none"> - In situ analysis 	<ul style="list-style-type: none"> - Improved analytical methods 	<ul style="list-style-type: none"> - In situ process control

Table II.3: Technological focus of catalysis in process optimisation

Roadmap Polymers and Materials

Sector Definition

Production of polymeric materials and composites for bulk and speciality industrial and consumer applications. Applications are to be found in structural materials, elastomers (rubbers), packaging, films, fibres, coatings, paints, glues and electro/optic materials. Polymers can be of natural or man-made origin (e.g. natural or synthetic rubber or fibres). The focus on catalysis limits the sector to organic-polymeric materials and composites thereof of man-made origin and addition polymers like polyethylene or polypropene rather than condensation polymers like Nylon or PET.

Sector in 2010

High performance polymeric materials will be produced in bulk based on a few cheap building blocks by means of selective catalysts, controlling microstructure and composition at will, including (stereo and compositional) block structures and blends. Production will be either very large scale and centralised, or small scale for local demand. Polymers with custom properties can be designed and produced. Nano-composites with improved physical properties will find wide application. Production processes will be essentially solvent-less (bulk, gas-phase). Materials will have controlled permeabilities, dyeability, and compatibility by controlled introduction of functionality's (also in alpha-olefins). Recycling/depolymerization will be practised for bulk polymers where appropriate.

Biodegradable polymers and polymers based on biofeedstocks will play an increasing, but relatively limited, role (medical applications, disposables). Conducting and functional polymers will be prominent in solar cell, battery, and electronic (semiconductor, photonic) applications. Fully waterborne systems and controlled polymerisation/drying/curing systems will be used for coatings and paints.

The above developments will be driven by the replacement of more expensive and heavier materials (especially metals) in structural and electronic applications. The demand for polymer performance and processing properties by users, and cost, will be the dominant factors. Other issues are environmental concerns and legislation (e.g. PVC replacement, degradability, elimination of volatile organic solvents), sustainability of feedstock supply (building blocks), requirements of new materials for medical applications, simplified processing, process intensification (molecular blending in single reactor, injection polymerisation and blending) and logistics (raw materials supply vs. polymer users).

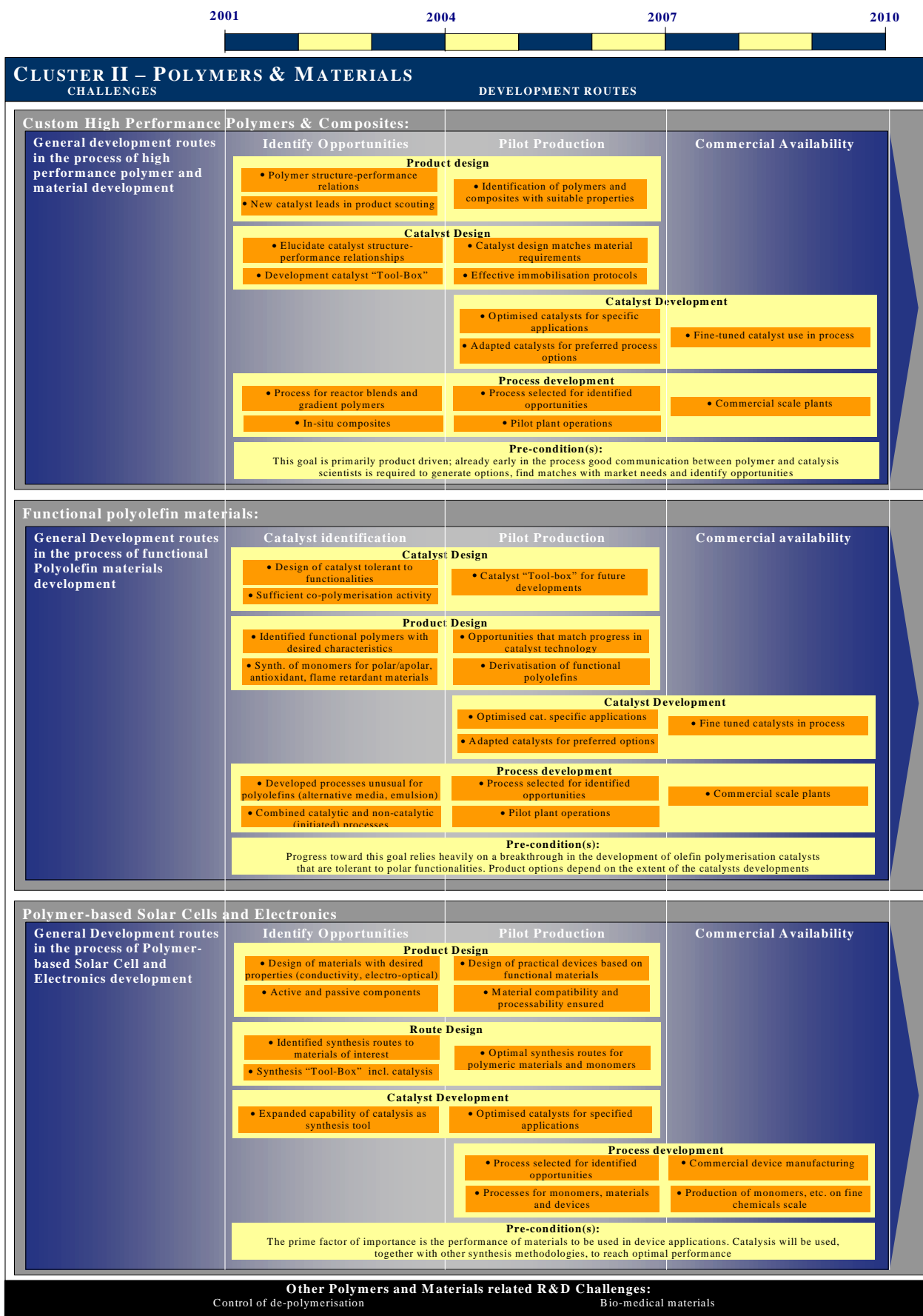
Overview of high-priority goals

- a. **High-priority goal 1: (100%) Tailor-made high-performance polymers and composites.** Optimal, fine-tuneable polymer properties in bulk and speciality polymers by catalysis.
- b. **High-priority goal 2: Functional polyolefin materials.** Random co-polymerisation of olefins with monomers with polar functionalities.

- c. **High-priority goal 3: Polymer-based solar cells and electronics.** Lightweight and flexible systems that can compete with inorganic-based technology.

Development routes

Picture II.5 provides an overview of the development routes in the Polymers & Materials sector.



Picture II.5: Catalysis in Polymers & Materials Roadmap

High-priority Goal 1: Tailor-made (high) performance polymers and composites

The ultimate goal in Polymers and Materials is the following sequence:

- Definition of desired properties
- Design of polymer (or blend/composite) based on an intimate understanding of structure/property relationships (molecular modelling)
- Selection of required catalyst(s) - based on the polymer grade to be made
- Dedicated manufacturing of desired polymer grade (flexible plants, localised manufacturing, “mini-mill” concept)

Control of polymer properties is important for all types of polymeric materials, especially for those materials with demanding specifications on one or more levels (e.g. mechanical properties, processability or electronic properties). The optimal use of the physical properties of polymers may be achieved by full control of polymer “molecular” properties, and by using the possibilities of (nano-)composites and reactor blends, for both bulk scale and speciality scale polymers.

Catalysis is an important means for polymer synthesis in general (and the only route available for many classes of polymers), and use of well-defined catalyst species allows for designed control of selectivity. Features to be controlled include stereo- and regioregularity, copolymer composition, random or block incorporation of co-monomer, molecular weight distribution, dispersion and adhesion of inorganic fillers/fibers, polymer morphology and processability.

The most economically important classes of polymer materials are polyolefins, polyesters, polyamides and polyurethanes. In addition, polymers with more diverse compositions, e.g. for use in electronics or for medical applications, will gain in importance. The largest family of the bulk-type polymers are the various polyolefins (polyethene, polypropene and copolymers) with their derived products: injection and blow-moulded products, films, fibers. These are all (except for LDPE) prepared exclusively by catalysis. A large quantity of these materials will continue to be made with existing catalysts, but new catalyst technology is required for new materials and products with highly demanding product specifications. This is especially important for the continued replacement of other (more energy-demanding and less environmentally friendly) materials by polyolefins. Good processability combined with the best possible product physical properties is required (e.g. highly defect-free polymer chains for fiber spinning). Extending the applicability range of a single polymer type is of importance, as blends from two different types of polymers and / or use of different types of polymers in a single application (such as a car) hampers recycling. It would be preferable to meet various needs by tailoring the structure of a *single* type of polymer (e.g. different grades of polypropene for upholstery, bumpers, dash boards in cars). This may be reached by full control of stereo-, regio- and sequence selectivity in the polymerisation.

Most polymers require various additives to improve UV stability, oxidative stability, processability, flexibility, and fire retardancy. These additives are blended in afterwards, a process which requires relatively high amounts of additives to get a proper dispersion of the additive through the polymer matrix. More efficient use of additives may be achieved by the incorporation of the additives by co-polymerisation of monomers containing the additive functionalities. This minimises additive leaching, improves recyclability and will require much lower levels of additives. To achieve this, catalysts capable of co-polymerising additive

molecules should be developed. Catalysts with properties suitable for this purpose in conjunction with polyolefins may also emerge from the area described in goal 3 (see below).

The use of composites is often cost advantageous, allows the use of less petrochemical (and thus finite) resources, and gives materials with better mechanical properties. Compatibility between the (two) components of the composite material is often a problem (*e.g.* polypropene and glass fiber). To make optimal use of the properties of composites, catalysts that allow the incorporation of functional co-monomers (which enhance compatibility) are highly desirable.

In many cases, reactor blends - simultaneous production of two types or two grades of polymers in a single reactor - can yield better materials than those obtained by blending of polymers afterwards. Production of these reactor blends will require either the use of a mixture of catalysts, which traditionally have different “operating windows”, or a single catalyst that can produce different grades of polymer upon changing the reaction conditions. To arrive at economically attractive production of reactor blends, catalysts need to be developed which produce different (grades of) polymers, yet can co-exist and have similar operating windows. The process engineering aspect of the production of reactor blends is also a challenging area.

Highly controllable polymerisation catalysis will also be important in realising the full potential of materials based on renewable resources (*e.g.* polylactide), if these are to make a significant impact in the future. The same can be said for the production of polymers for electronic applications (which have very high requirements with respect to their physical properties and purity). Coherent progress in this area will require a good combination of efforts in polymerisation catalyst development and catalyst immobilisation, polymerisation process engineering and polymer structure-property research.

Technological focus of catalysis in this goal is:

- a. Mechanistic Investigations:** To reach the required control of catalytic polymer synthesis, a good basic understanding of the catalyst and process features that determine polymer properties is required. This means that both “exploratory” and “explanatory” research efforts are needed. A thorough understanding of catalyst structure-property relationships needs a good collaborative effort between experimentalists and theoretical chemists. The “focused exploratory” (lead evaluation/optimisation) research should benefit greatly from the use of parallel synthesis/ rapid screening techniques. To ensure a good focus and an efficient development, it is essential to make a sound choice of the polymer materials classes to be targeted (especially those where the physical properties ensure new or increased commercial opportunities). The application of this catalysis technology in processes also depends on other factors, such as the successful immobilisation of catalysts on supports with retention of catalyst properties. For gas phase and slurry phase processes (morphology control) this is essential for practical application. The production of reactor blends obviously has catalyst as well as process technology aspects.

b. Development targets:

- **Ligand controlled polymerisation, catalyst structure performance relationships**
Primarily (but not exclusively) polyolefins and polymers made via ring opening polymerisation's (lactide, epoxide, epoxide/CO₂)
- **Good targets for polymers made from renewable resources**
- **Catalyst immobilisation** methods and supports, also applicable to (nano-)composites

Technologies in “Tailor-made (high) performance polymers and composites”

The development routes in this high-priority goal are generic. The technological focus of catalysis is therefore also generic in relation to the R&D-areas.

Catalyst Design & Discovery

- Mechanistic investigations
- Catalyst modelling (QM/MM)
- Ligand design and synthesis
- Catalyst immobilisation

Catalyst Production

- Catalyst optimisation (Mw, copolym., activity, stability)
- Simultaneous screening of catalyst performance and polymer properties

Process Design

- Processes for reactor blends (single/multi reactor)
 - Processes for gradient polymers
- Gas-phase, liquid pool and HT solution processes
 - Kinetics and morphology modelling

Process engineering

- Dedicated smaller scale reactors
- Multi-purpose reactors

Process Monitoring & Control

Table II.4: Technological focus of catalysis in tailor-made (high) performance polymers and composites

High-priority Goal 2: Functional polyolefin materials.

Goal is synthesis of novel (crystalline as well as amorphous) materials in which apolar and polar functionality's can be varied at will (random, in blocks), for controlled compatibility, dyeability and permeability properties as well as for the use of alternative feedstocks. The existing efficient olefin polymerisation catalysts are incompatible with polar functionality's (leading to rapid catalyst deactivation). Emerging classes of catalysts may offer a possibility for co-polymerisation of olefins and functionalised substrates to make these materials accessible.

Products of this nature will be highly valuable as compatibilisers, dyeability improvers and for use in coatings, as well as for providing new materials with specific permeability properties. Medical applications are also foreseen. Many desirable materials that fall in this class, such as linear random co-polymers of ethene and acrylate, are presently inaccessible. Success in finding catalytic routes to such materials will thus spur a “materials discovery” research process. Products are expected to have a high added value.

Catalysts that are tolerant to polar functionalities should also be suitable for the co-polymerisation of co-monomers that bear antioxidant, flame-retardant, compatibilising or self-repairing functionalities. These materials will be useful to enhance the performance of bulk polymers, and will minimise problems with additive blending and leaching.

In addition, the trend that monomers made from bio-feedstock may become more important has two implications for desired catalysts:

- Existing monomers produced from bio-feedstocks are more likely to contain (polar) impurities (such as water, sulphur containing compounds, CO₂), which may act as catalyst poisons.

Thus, more robust catalyst are required.

- “New” monomers with polar functionalities may become available - catalysts that can tolerate/process such monomers are needed.

Technological focus of catalysis in this goal is:

- Development of polymerisation catalysts** that effectively polymerise and co-polymerise olefins and that are tolerant to a wide range of polar functionality’s (esters, nitriles, alcohols) is the main task. Over the past three years interesting leads have emerged in late transition-metal based catalysts, but the ultimate goal is still out of reach. An energetic catalyst research effort should be able to bring this closer to realisation. In addition, interesting materials with properties of interest for these applications may be obtained by combining catalytic and non-catalytic (ionic, controlled radical) polymerisation routes, although process disadvantages over fully catalytic routes exist.
- Development targets are:**
 - **Functionality-tolerant olefin polymerisation catalysts**, likely based on late transition metals.
 - **Interaction with polymer property scientists** to define ‘intermediate’ goals for potentially useful materials/co-monomers.

Technologies in “Functional polyolefin materials”

The development routes in this high-priority goal are generic. The technological focus of catalysis is therefore also generic in relation to the R&D areas.

Catalyst Design & Discovery

- Mechanistic investigations (catalyst-substrate interactions)
 - Catalyst modelling (QM/MM)
 - Ligand design and synthesis

Catalyst Production

- Catalyst optimisation (stability, copolym.)
- Screening of catalyst performance and product properties

- Process Design

- Alternative process media
- Solution, slurry and emulsion reactors
- Post-polymerisation reactions

Process engineering

Process Monitoring & Control

Table II.5: Technological focus of catalysis in Functional polyolefin materials

High-priority Goal 3: Polymer-based solar cells and electronics. Lightweight/flexible systems that can compete with inorganic-based technology.

The design and production of devices (electronic, electro-optic, etc.) based on polymers that can compete with inorganic materials is of great interest. Examples are flexible electronic circuits and displays, and light-weight photovoltaic cells. Of prime importance are the active component materials, of which the actual electronic and optical properties allow the devices to function. The means of production of these materials (including the precursors or building blocks) is as yet secondary. Nevertheless, successful devices need to be mass-produced eventually, and catalytic synthesis of materials has a number of important advantages (selectivity, waste reduction) over non-catalytic synthesis. An additional issue is the high level of chemical purity that is usually required for these active components (also implying that catalyst remains should be minimal or inert). Another aspect of polymer-based devices is the support and protective overlayer material. This should provide sufficient protection/robustness, yet allow ready processing of the devices.

Catalysis can also be applied to one particular step in a multi-step materials synthesis process, or in the clean and efficient synthesis of the required building blocks. This aspect is closely related to the Fine Chemicals sector. It needs to be determined where catalysis can assist in the materials synthesis in this emerging application area as well as in the materials discovery process.

Polymeric products that are important to this group of applications are: conducting and semi-conducting polymers, non-linear optical and waveguide materials, photoactive materials (for light capture and charge separation), light-emitting materials, materials with tuneable band-gaps, etc. Of relevance are also the techniques that are used in device fabrication. The products should be suitable from both the properties and the processability aspects.

The technological focus of catalysis in this goal depends greatly on the materials deemed most suitable by device scientists. In this area it is not so much that catalysis is generating new materials, as well as efficient means of preparing the materials of choice. For this, it is essential that a better contact is established between the relevant scientific communities. This will be important in the long run, as this will be a strongly developing area.

Technologies in “Polymer-based solar cells and electronics”	
The development routes and the technological focus of catalysis are generic for the R&D areas.	
Catalyst Design & Discovery	<ul style="list-style-type: none"> - Catalysed polymer synthesis (insertion and RO(M)P polymerisation) - Initiated polymerisations (ionic, controlled radical) - Catalysed organic synthesis
Catalyst Production	<ul style="list-style-type: none"> - Catalyst optimisation (High selectivity, highly pure products) - Catalyst performance and product screening
	- Process Design
Process engineering	<ul style="list-style-type: none"> - High purity monomers and materials - Fine-chemicals scale (multi-purpose reactors)
	- Process Monitoring & Control

Table II.6: Technological focus of catalysis in polymer based solar-cells and electronics

Roadmap Detergents and Textiles

Sector Definition

Based on the “Vision & Goals” workshop a third sector was appointed as relevant to the cluster besides the sectors Bulk Chemicals and Polymers and Materials. This third sector comprised areas like detergents, paper and pulp, leather, and textiles, which all have the use of water as process medium in common. Due to the lack of participation of catalysis experts from these sectors in the workshops and the fact that the TRM-core team did not have the expertise, it proved hard to cover this sector as extensively as the other sectors of this cluster. No detailed information could be obtained on the role of / trends in catalysis in paper and pulp and leather areas. More information was available for the detergents and textile areas, hence the sector was named after these. However, even for these areas expertise and manpower were hard to find and consequently, our analyses were less elaborate.

This section of the roadmap has been included as a broad overview of the sectors. Aim is identification of areas in which catalysis could play a role without providing development routes and technological detailing.

The Detergents sector

The Detergents sector is concerned with production of detergent formulations for household cleaning globally. Heavy-duty detergents consist mainly of surfactants (often derived from petrochemical sources; sulfonate or carboxylate-containing surfactants), zeolites or triphosphates for binding of calcium or magnesium ions from tap water, enzymes (proteases, lipases, amylase) to remove a variety of mainly food stains, such as fatty stains or egg yolk, and bleaches (Tetra Acetyl Ethylene Diamine (TAED) / percarbonate) yielding peracetic acid and hydrogen peroxide as bleaches. Bleaches are important for removing a variety of stains.

The Textiles sector

The Textiles sector involves the production of textile materials for industrial, consumer, safety, agricultural and medical applications. Additional applications are geotextiles and materials for the automotive and aircraft industry. Textile materials can be of natural or man-made origin (natural or synthetic fibres). Besides the production of structured materials from fibres the application of new (synthetic) fibres (with e.g. different permeability and dyeability), coatings (e.g. flame retarding agents, water repellence), laminates and new or more efficient pre-treatment and finishing processes (e.g. coating, dyeing, printing, sizing, bleaching, scouring) is of importance for the (Dutch) textile industry.

Sector in 2010

The Detergents sector

Cheap detergent products which offer improved bleaching efficiency through the use of (bio)catalysis, requiring less water per washing cycle and operating at lower washing temperatures will be available to serve global needs.

The Textiles sector

In 2010 textile production processes will have become more sustainable by having reduced consumption of energy, water and chemicals through the use of (bio)catalysts in and better process integration of the sizing, scouring and bleaching steps. In addition, biopolymers, advanced coatings and laminates are expected to become increasingly important.

Overview of high-priority goals

As discussed earlier the Detergents & Textiles sector was elaborated in less detail than the other sectors. For the sectors we see as an overarching theme:

High-priority Goal 1: “Sustainable Oxidation in Aqueous Environment”.

Sustainable oxidation in aqueous environment is definitely a topic that concerns this sector; examples are bleaching processes in the textiles and detergents sectors. It is however, less clear what the role of catalysis in achieving this goal can and will be. For the detergents and textiles sectors to enhance the low temperature efficiency of bleaches and to reduce consumption of energy, water, and chemicals, use of transition metal catalysts or perhaps (per)oxidase enzymes is an avenue that might be pursued. The choice of the metal ion is highly motivated by environmental constraints. Bleach catalysts can also be employed at low bleach levels, thereby reducing the chemical loading and allowing more consumers to use the efficient bleach technology.

Goal related products/processes for each of the sectors are:

- a. **Detergents.** There are several drivers to make detergents globally more efficient. Most consumers world-wide do not own or have access to washing machines to clean their clothes at the desired temperature. Besides, most consumers cannot afford detergent products containing bleaches that are very expensive. As the world's fresh water supply is limited the amount of water per wash cycle will have to come down. Finally, especially in the EU, the washing temperature to efficiently use the bleaching technology is quite high (> 40°C). Using a more efficient bleaching technology will allow a further decrease in the average washing temperature. It is foreseen that the enzymes already used in the current detergents play a more important role, including perhaps novel enzymes to yield a wider/better stain removal. To enhance the efficiency of bleaches, it is expected that the use of transition-metal catalysts or perhaps (per)oxidase enzymes will enable efficient use of detergents at low temperature. The choice of the metal ion is highly motivated by environmental constraints. Bleach catalysts can also be employed at low bleach levels, thereby reducing the chemical loading and allowing more consumers to use the efficient bleach technology.

b. Textiles. It is expected that textile production processes will be shifted substantially towards sustainable processes, within 10 years, due to increasing governmental and environmental restrictions and the availability of fresh water. The present focus in research, innovation and development is mainly the sustainability, efficiency and intensification of different chemical, physical and biotechnological textile pre-treatment and finishing processes. Biocatalysis is a promising technology to meet the expected future requirements.

In the present bleaching and scouring processes the temperature is rather high (50-100°C). Thereby these processes need high concentrations of chemicals that are not reused. Catalysts and biocatalysts can be employed at low concentrations, thereby reducing the chemical loading. Enhancing the efficiency of bleaches, using transition-metal catalysts or (per)oxidase enzymes might enable the industry to use lower temperatures. It is foreseen that the scouring process will be improved using e.g. pectinases or cellulases. A more efficient bleaching and scouring technology will enable the industry to decrease the energy and water consumption. Besides no chemicals will be necessary for neutralisation, and the amount of waste water produced will decrease. It is expected that enzymes will play a major role, especially since enzymes could allow different processes to be integrated (e.g. sizing, scouring and bleaching). A reduction in process steps will cause a significant decrease in energy and water consumption, since in the present situation rinsing is necessary between most treatments.

Biopolymers, advanced coatings and laminates are expected to play an increasingly important role. The expected developments will act as a stimulus for the textile industry and may improve existing processes and introduce new, more efficient and environmentally fully acceptable processes and advanced materials with special properties.

The technological focus of catalysis in these sectors is mainly the more efficient bleaching steps in the textiles and detergents areas where there is ample need for more robust and cheap biocatalysts or cheap, non-toxic man-made catalysts.

Development Routes

Due to the lacking expertise in the workshops and the TRM Catalysis core team it has not been possible to generate development routes and technological detailing for the Detergents and Textile sectors.

5. CLUSTER III: FINE CHEMICALS, PHARMA AND FOOD & FEED

Introduction to Cluster III

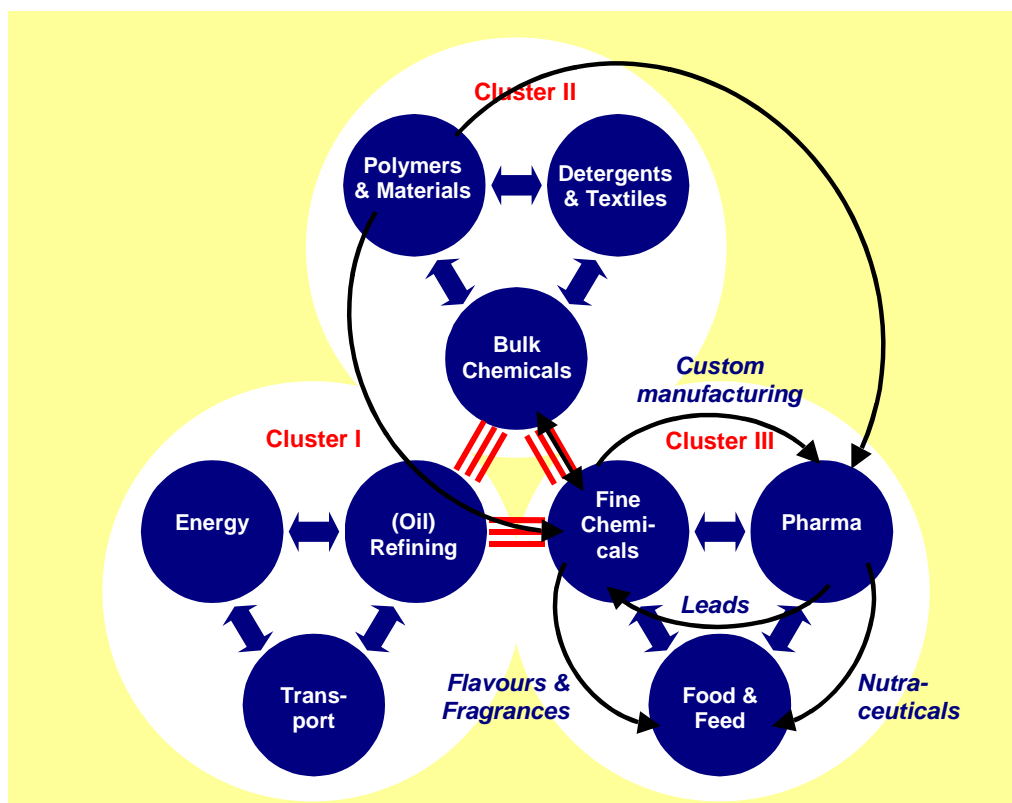
Cluster III comprises the Fine Chemicals, Pharma, and Food & Feed Sectors.

The cluster utilises the complete spectrum of catalysis, involving heterogeneous, homogeneous, as well as bio-catalysts. The Fine Chemicals area is a bridging sector between bulk and life sciences. Larger-scale production of e.g. lubricants, speciality detergents and corrosion inhibitors is found here, as well as kg-scale synthesis of chemicals for pharmaceuticals. This implies that there are quite different driving forces within the cluster. While in the larger scale Fine Chemicals area it is largely the price that is important, in the pharmaceuticals area factors like stereoselectivity and purity, but also quick response to a given synthetic problem are much more important. The cluster is further characterised by the strong tendency to move from stoichiometric to highly selective catalytic reactions (chemo-, regio- and stereoselective). Beside the improvement of “classical” catalysts (chemo- and bio-) a strong future push can be expected from the integration of disciplines. In contrast to catalytic processes for commodities, the catalytic processes of this cluster have to be developed fast and are mostly not optimised with respect to catalyst use and costs. Process development in Cluster III requires flexibility and is carried out in multi-purpose production plants.

An issue that is important in all three sectors of this cluster (but most important in the Food & Feed sector) is the public acceptance of recombinant DNA technology.

Relations between the clusters

It is evident that the sectors in this cluster have strong interrelations. The Pharma sector defines to a good portion the demands for the Fine Chemicals sector. In addition, the sectors Pharma and Food & Feed are related in the area of nutraceuticals development. Fine Chemicals and Food & Feed are linked through the use of catalysis for the development of more efficient routes to flavours and fragrances. The sectors profit collectively from developments in the specifically required technology fields, even though the detailed objectives for which the technology is used may differ. Despite the different application areas, the knowledge on catalyst properties and technological use (catalyst toolbox) can be shared between the three sectors.



Picture III.2: Relations between sectors as seen from a cluster III perspective.

Outside of the cluster, the reactor technological aspects of the Fine Chemicals sector have a link to the Bulk Chemicals area, especially concerning the desired high degree of transferability from development to production scale. The sectors Polymers and Materials of Cluster II and Pharma could interact where medical devices for diagnosis and drug dosing systems are concerned. In addition, the developments in the sector Polymers and Materials of Cluster II could result in materials for catalyst immobilisation and new membrane materials that may be of use in the Fine Chemicals sector.

Roadmap Fine Chemicals

Sector Definition

Sector bridging bulk chemicals and small-scale specialities, typically chemicals produced below a volume of 10,000 ton per year per production site.

Sector in 2010

The main issue will be a considerably reduced time-to-market driven by requested quick-response production of compounds and materials. New reactor concepts and the replacement of most classical routes by more efficient and highly selective catalytic processes allow a waste reduction of at least 50%. More complex and highly pure chemical entities will be demanded by the pharma industries. Products are made with a high degree of chemo-, regio- and stereoselectivity. An important trend in this field is the introduction of so-called cascade catalysis, where several transformations will be performed in one single process step. Development time is shortened by massive use of parallel and combinatorial screening and testing methods. Biocatalysis is increasingly used in addition to and in combination with other means of catalysis (also for products of >2000 ton per year), especially in food, feed and drug applications. Biocatalysts are tailored towards non-natural process conditions by *ex-vivo* laboratory evolution techniques. High and ultra-high through-put screening methods are combined with methods to generate biological diversity. Miniplant and microplant technology makes a small-scale production in continuous operation possible, which gives intrinsic advantages with regard to safety. Considerable attention will be paid to direct scale up from laboratory to production plant.

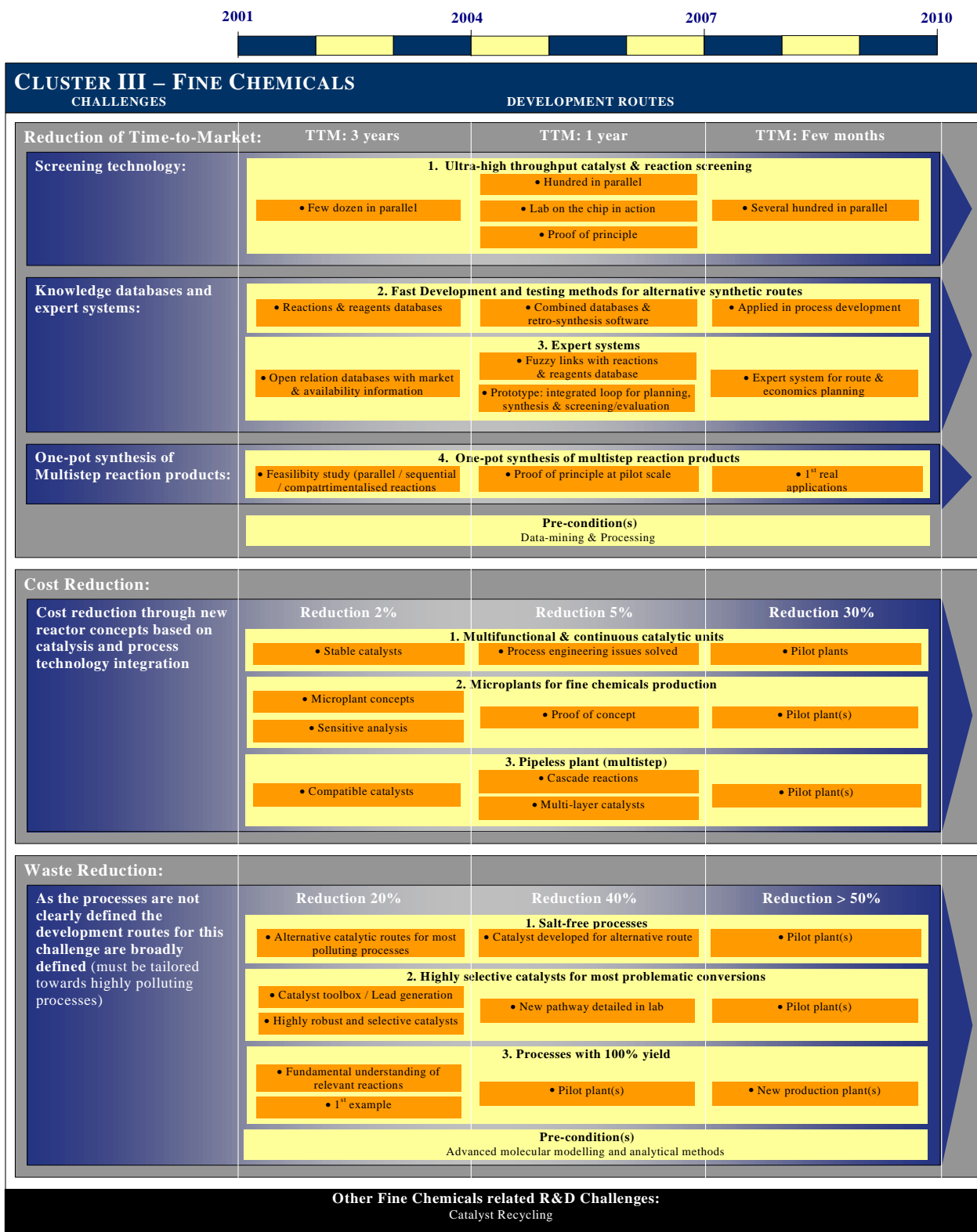
Overview of high-priority goals

The high-priority goals as defined in the “Vision & Goals” workshop in the Fine Chemical sector are:

- a. **Reduction of time-to-market** of 50%
- b. **Cost price reduction** through new reactor concepts such as:
 - Pipeless plant (first commercial applications)
 - Microplants with 100% transferability from laboratory to production scale
 - Introduction of multifunctional continuous units
- c. **Waste reduction** in process of at least 50%

Increasing the overall selectivity of the processes (which should be 100% for novel processes) will be of great importance for all of the 3 goals mentioned, but especially for the waste problem. Selectivity is therefore not a separate item. The term Cascade catalysis means the combination of several transformations in one process step.

Development routes



Picture III.3: Catalysis in Fine Chemicals Roadmap.

High-priority Goal 1: Reduction of time-to-market

Fine chemicals production does not deal with the invention of new products, this part has been completed before it goes to production. In this phase, the desired end product is known and the goal is to produce it, or to produce an intermediate with the required purity in the fastest possible way. The main forwards and conditions are given in the sector description part above.

Development routes related to the reduction of Time-to-market in the fine chemicals are:

- a. **Screening technology:** Development routes in this area include:
 - **Ultra-high through-put catalyst & reaction screening:** For a fast development of new processes it is highly desirable to find the right catalyst for a certain conversion in a very short time. Beside the ability to prepare, test and analyse many catalysts at the same time, this requires a catalyst tool-box with the collective knowledge about catalysts for specific reactions, their chemistry, substrate range, physicochemical properties and kinetics of typical (as much as possible) reactions. Not only the catalyst has to be found, but also the right reactor type and the corresponding engineering. This requires an integration at an early stage of testing, preferably on the level of high-throughput experimentation.
- b. **Knowledge databases and expert systems:** Development routes in this area include:
 - **Fast development and testing methods for alternative synthetic routes:** A desired product in the Fine Chemicals area is most likely derived from a multi step sequence of conversions. Working out such whole sequences has to be speeded up considerably. This requires collective retrosynthetic expertise and information about availability of building blocks.
 - **Expert systems:** An expert system for this area should ideally combine all of the aspects mentioned above and automatically work out a number of most likely synthetic routes based on a database of conversions, the availability of building blocks inside a company or commercially, and financial information about substrate and catalyst costs. In this way it should be able to come up with a few suggestions, such as:
 - Selection of building blocks and check for availability in company and/or commercially
 - Retro-synthesis (to determine possible routes)
 - Calculate alternatives based on data in databases
- c. **One-pot syntheses for multi-step reaction products:** In view of the trend to process intensification, combining several conversions and separation steps in one unit, there is a strong need for new synthetic routes. Retrosynthesis with special emphasis on the multidisciplinary of the design process has to be employed, including organic chemistry, biochemistry, process technology, catalyst-technology and informatics. There is a strong need for knowledge about catalyst compatibility. This holds for multi-metallic, multifunctional catalysts, but also for mixtures of enzymes and cofactors and mixtures of biocatalysts and metalcatalysts.

The technological needs related to reduction of time-to-market are mainly related to fast screening of catalysts and reactions. Key element will be to develop a toolbox for classification and screening of catalysts for specific conversions. Such a catalysis/bio-catalysis toolbox will include:

- Cells, enzymes, homogeneous and heterogeneous catalysts
- Knowledge on reaction types and conditions which will include molecular technology, computational chemistry, functional genomics, genome mining and enzyme evolution.

Three different steps in the development of the Toolbox are foreseen, which will be tackled in parallel. As soon as new catalysts become available, these should be tested and added to the library. In this way, a toolbox is continuously built up and improved, while knowledge is collected. Activities are:

- **Grouping into reaction types and set-up of libraries for testing**
- **Testing:** Faster testing and analysis of reaction-mixtures on a small scale. For homogeneous the aim is development of more specific test methods and measurements in parallel (increased numbers). Screening should be on smaller scale, more specific and more sensitive.

Technologies related to this are:

- Analysis: HTS / MS / HTS NMR / GCMS / LCMS
- Hardware and software: automated data handling and data-mining

In existing technology incremental changes and gradual improvements are expected. For new technologies (Raman, Laser, IR and NMR), step changes are expected. Short-term focus will be colour reactions (100 per day) to 10,000 per day in the medium long term.

- **Validation of libraries & possibly building up of expert systems**

Technologies in reduction of Time-to-Market			
1. Ultra-high through-put catalyst & reaction screening	2. Fast development and testing methods for alternative synthetic routes	3. Expert systems	4. One-pot synthesis of multistep reaction products
Catalyst Design & Discovery			
- Directed evolution, immobilisation			- Compatible catalysts, multilayer/compartmentalised catalysts
Catalyst Production			
Process Design			
- Miniaturisation, robotics	- Databases and evaluation tools	- Databases and evaluation tools	
Process engineering			
			- Advanced process control
Process Monitoring & Control			
- Fast and detailed microanalysis	- Fast and detailed microanalysis		- Multi parameter in situ analysis

Table III.1: Technological focus of catalysis in reduction of time-to-market

High-priority Goal 2: Cost reduction

The integration of catalysis and process technology is the key to reduce costs. This goal comprises a/o continuous process – pipeless plant / one pot / multistep, 100% transferability or parallel working micro plants. Goal related development routes are:

- a. Multifunctional & continuous catalytic units:** A paradigm has been broken, that is, that fine chemicals below a production capacity of ~ 5000 ton per year and plant are preferably produced in multipurpose batch reactors. The ability to run homogeneously catalysed reactions in a continuous fashion will bring about considerable reaction engineering advantages. A strong technology-push is expected in this area from analytical techniques, the immobilisation of homogeneous catalysts, connected with supramolecular approaches and developments in membrane technology and new reaction media.

Technologies needed are:

- **Integration:** Small-scale processes can continuously be carried out in plants, that can be used in a flexible way. Clear advantages to the batch process will have to be shown case-by-case.
- **Separation:** Catalysts have to be recycled/kept inside the reactor
 - Immobilisation of existing catalysts (optimisation of existing technology, development line)
 - Supramolecular approach, completely new developments (new dev. steps)
 - Existing **and new membrane materials** for ultra- and nano-filtration
- **Multilayer systems, new solvents** – relation with pipeless plant (magic ball) and membrane technology

- b. Microplants for fine chemicals production:** The use of microplants for production brings a number of advantages, starting with security aspects. The production methods of this kind of equipment (etching) makes the units cheap and allows the use of dedicated continuous units for small-scale production. Production can be more efficient and market oriented in place of batch production and need for storage nowadays. This sector will develop along with the advances in miniaturisation and analytical methods (small scale testing).

Microplant technology is regarded to make processes safer, introduce more control and more flexibility in production.

Technologies needed are:

- **Sensitive measurement and analysis techniques** are a prerequisite, esp. the analysis of traces of (by)products.
- **Precise modelling and understanding** is important, the development of hydrodynamics / kinetic modelling of catalysts / determination of mass and heat balances on microscale / computational chemistry. Miniaturisation of analytical techniques; online/ faster =>complete analysis
- **Input of reactor technology.** Development of new concepts and change existing concepts for the specific needs in fine chemicals area

c. Pipeless plants (multistep): In connection with the trend towards process intensification it is desirable to carry out a sequence of reactions and separation steps in one unit. Therefore knowledge is needed on the influence of one reaction/catalyst on another. Integration of bio-catalysis and chemical catalysts has to be put forward to develop new kind of processes (e.g. deracemisation). In order to achieve compatibility where it is not intrinsically reachable, the design and application of the catalysts have to be adapted (a/o immobilisation, multilayer systems, micellar/unimolecular micelles (magic ball)). Separation technology (membrane technology, separated compartments in a reactor) will have a strong impact in this field. Toolbox – knowledge of catalysts and interaction between them; operational windows (partially matches the catalyst-toolbox).

Characteristic is the combined execution of a series of reactions in the same reactor, including separation steps where possible. The ideal situation is a process where all compounds are fed into one reactor and the pure product comes out. Work-up and recovery of catalyst and cofactors should be included. (However, in many cases a deliberate separation of process steps may be cheaper, cleaner, more flexible, etc., as a result of which pipeless plants are not desired). Whole cells may be regarded as pipeless plants, and may be exploited as such, or they may inspire the development of non-living pipeless plants.

Technologies needed are:

- **A very efficient retro-synthesis and determination of suitable reaction sequences** is essential.
- Studies have to be carried out on the **compatibility of enzyme/enzyme systems, enzyme/catalyst systems and catalyst/catalyst systems**. This will lead to a toolbox or expert system for the planning of one-pot processes. For a specific case, yet to be chosen, this development will have to be undertaken and knowledge collected.
- **Precise measurement and process control/technology** will be crucial

Technologies in “Cost Reduction”		
1. Multifunctional & continuous catalytic units	2. Microplants for fine chemicals production	3. Pipeless plants (multi-step)
Catalyst Design & Discovery		
- Catalyst Stability		- Catalyst compatibility - Metabolic modelling
Catalyst Production		
		- Multilayer catalysts
Process Design		
- Multifunctional reactor concepts	- Miniaturisation / Robotics	
Process engineering		
- Catalyst Immobilisation - Separation	- Kinetic Modelling	
Process Monitoring & Control		
		- Sensitive Analysis

Table III.2: Technological focus of catalysis in cost reduction

High-priority Goal 3: Waste reduction in process

This goal is extremely broad as the processes are not clearly defined. The focus lies on the most polluting processes. As waste reduction usually involves increasing atom efficiency, costs-reduction will be achieved as well (High-priority Goal 1). Goal related development routes are:

- a. Salt-free processes:** The production of effluent salts in fine chemicals production has to be circumvented. Catalysts (enzymes) have to be optimised for working at other pH (neutral). The use of organic solvents has to be reduced extensively. Organic solvents need to be replaced by water as the solvent where ever possible. This needs to be realised at a relatively short term.
- b. Highly selective catalysts for most problematic conversions:** Catalysts are needed that are very selective (stereo- / chemo-) and whose lifetimes are increased extensively (through work up / recycling). In addition, catalysts need to be able to operate at moderate temperatures (ideally room temperature). The (heavy) metals used also need to be evaluated and some may have to be banned. Catalysts also have to be discovered faster (similar to pharma). Catalysts are improved continuously, but major improvements (e.g. selectivity) are expected on the medium long term.
- c. Processes with 100% yield:** Process waste converted into a product.

Technological needs related to these development routes are strongly related to the process. Steps that need to be followed are:

- Selection of the most polluting processes and identification the critical step;
- Develop alternative routes/reaction pathways. This is strongly related and largely identical to what was mentioned before within Fine Chemicals, at Reduction of time-to-market. Analytical techniques and high throughput screening methods are needed;
- It is important that in case of existing products (pharma) no new by-products or impurities are introduced (testing and admittance);
- Scale up

Technologies in “Waste Reduction”		
1. Salt-free processes	2. Highly selective catalysts for most problematic conversions	3. Processes with 100% yield
Catalyst Design & Discovery		
- Catalyst toolbox	- High-throughput	- Toolbox
- High-throughput	- Catalyst optimisation	- Catalyst optimisation
- Reaction database	- Modelling & toolbox	- Selectivity & stability
		- High throughput
Catalyst Production		
Process Design		
- Process concepts	- Integration & intensification	
Process engineering		
Process Monitoring & Control		

Table III.3: Technological focus of catalysis in waste reduction

Roadmap Pharma

Sector Definition

Discovery, design and production of compounds, materials and devices for applications in medicine.

Sector in 2010

In 2010 a more diverse portfolio of pharmaceutical products, which are both much more selective and active (reduced side effects), is used. Analytical procedures are more elaborate and precise (including metabolite measurements, enzyme level determinations, gene chips and genome analysis) and allow a more reliable diagnosis. Patient-specific drugs that fit these diagnostic profiles are available. There is a trend to the development of pro-active drugs (prevention), enantiomerically pure pharmaceuticals and structurally more complex drugs. Drugs for gene therapy constitute a significant part of the market and cell therapies are used to cure rather than treat. Drug discovery is faster and more specific, making use of high through-put synthesis and ultra high through-put screening techniques. Production of intermediates for the synthesis of drugs is largely done in the Fine-Chemicals sector, which is aiming at production at an early stage of the development. The Pharma sector mainly focuses on drug discovery, but is also involved in especially the later steps in drug synthesis, where quality is of primary importance (cGMP, free of pyrogens etc.). New materials are used for drug delivery systems (e.g. slow drug-release) and biocompatible materials for construction of artificial (implantable) organs.

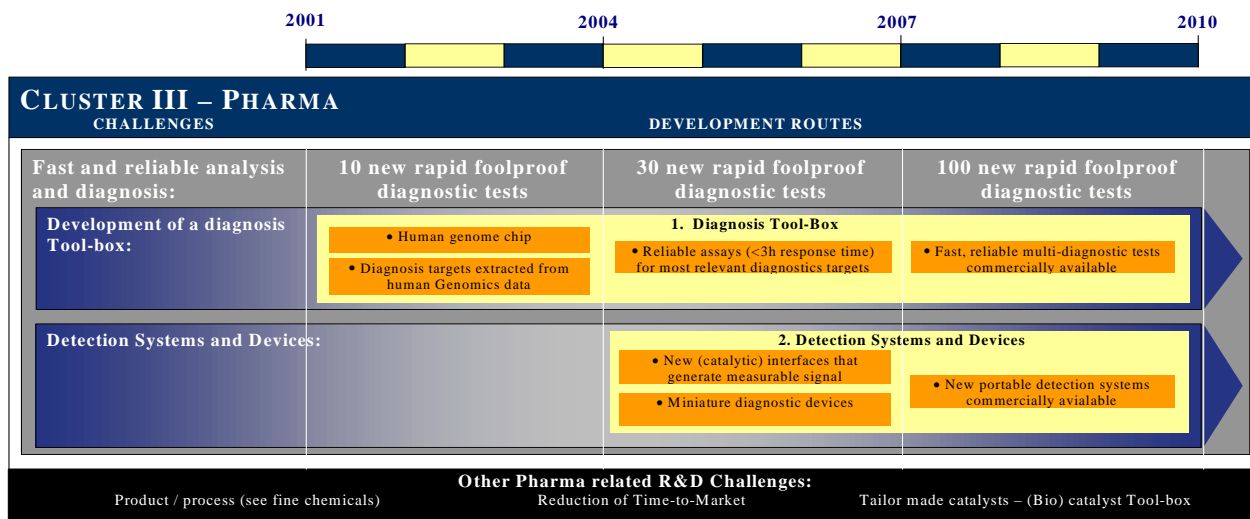
Overview of high-priority goals

The high-priority goals with respect to catalysis of the Pharma sector largely coincide with those of the Fine Chemicals sector: reduction of time to market, costs and waste. The supporting technologies and development routes are similar as well, despite the differences in boundary conditions such as costs and quality demands. Therefore, catalysis in the synthesis of drugs, although it is recognized as part of the Pharma sector, is treated in the sector Fine Chemicals.

A catalysis area that is specific for the Pharma-sector is “diagnostics and analysis”, which in a broader context could be considered as “catalysis in analytical methods”, and is of relevance to the majority of the other sectors as well. The high-priority goal that is specific for catalysis in Pharma therefore is: **Fast and reliable analysis and diagnosis**

Topics such as the use of catalysis for the development of new administration forms, i.e. the slow or targeted release of medicine is to be included in the Sector Polymers and Materials and will not be worked out here.

Development routes



Picture III.3: Catalysis in Pharma Roadmap.

High-priority Goal 1: Fast and reliable analysis and diagnosis

Diagnosis is a difficult task in medicine with the risks of misdiagnosis, not detecting a disease at all or detecting it at too late a stage. Developing knowledge on the causes of a disease at the genetic and biochemical level is a medical issue, but once the cause of a disease has been identified, selective screens to find new active compounds can be performed. This knowledge can also be used to reliably diagnose a disease, provided that a relevant metabolite or protein can be measured. A diagnosis toolbox, consisting of specific (bio)catalysts, can be employed to detect metabolites (e.g. using enzyme assays) or other compounds (e.g. using methods to detect interactions such as antigens/antibodies). This diagnosis toolbox can also be employed to develop detection methods for non-pharma applications, e.g. for quality control in the Food & Feed sector. The detection should be fast, reducing the time for diagnosis/analysis to minutes, especially in cases where this takes hours or days at present.

Goal related development routes are:

- a. **Diagnosis toolbox:** Development of diagnosis targets. The rapid increase in biochemical and the functional genomics data will assist in identifying target molecules for diagnosis. Similar to drug discovery screening, a diagnosis toolbox should be developed that allows the discrimination between cellular signals that are linked to the occurrence of a disease. Binding (RNA-DNA, protein-protein, protein-ligand or protein-antibody) and metabolite or (analogue) conversion, coupled to (catalytic) interfaces that translate these reactions in a generally measurable signal (e.g. electrical current, colour change, light emission), can be used. Both qualitative and quantitative measurements will be required.
- b. **Detection systems and devices:** Detection of a signal in blood and other fluids that corresponds to the occurrence of a disease can proceed inside (*in vivo*) and outside (*ex vivo*) of the body. *In vivo* detection systems should be biocompatible (both the materials and the detection system itself) and miniaturised (implantable). Catalysts that are used (frequently enzymes) should be compatible with interfaces that translate the reaction into an electronic signal (example: glucose oxidase can be used to measure blood glucose levels via an electrode). The amount of enzymes that is

currently available for such tests is limited (estimated at less than 10) and should be increased to be able to measure most common diagnosis metabolites (estimated at 100). Suitable *ex vivo* detection systems are similar, but need not to be miniaturised to the same extent (portable).

Technological needs related to these development routes are related to the use of catalysts in diagnosis (“catalysis in analysis”). The catalysts should selective, sensitive and fast. Frequently enzymes are used for this purpose, but the amount of available systems is limited. Genome mining and functional genomics information can be used to gain access to new detection reactions for diagnosis (conversion). Protein levels that cannot be measured in an assay could be analysed via binding (receptors, antibodies) or molecular characteristics (proteomics, Maldi-TOF MS). Lastly, gene chips can be used to detect RNA species that are specific for the development of a disease (transcript mapping). It should be considered to look for synergy between the catalysis field and the genomics programmes that are currently being built up in The Netherlands.

Technologies in “Reduction of aromatics”	
1. Development of a diagnosis toolbox	2. Detection systems and devices
Catalyst Design & Discovery	
<ul style="list-style-type: none"> - Supportive information technology: molecular modeling / bio-informatics / functional genomics - Directed evolution - High through-put experimentation 	
Catalyst Production	
<ul style="list-style-type: none"> - Catalysis / biocatalysis toolbox 	<ul style="list-style-type: none"> - Catalysis / biocatalysis toolbox - Catalytic interfaces
Process Design	
Process engineering	
	<ul style="list-style-type: none"> - Analysis hardware: miniaturisation / robotics
Process Monitoring & Control	

Table III.4: Technological focus of catalysis in reduction of aromatics

Roadmap Food & Feed

Sector Definition

Conversion of (agro) feedstocks to human/animal food and/or food additives.

Sector in 2010

More fundamental knowledge will be available concerning the relation between molecular structures and food properties. The interest in the well-being of humans increases. Low (no) calorie food remains important. New compounds will be added to food. The borderline between food and pharmaceuticals becomes blurred. In 2010 the food/feed sector may still face the problem that new products may be unacceptable for the consumer if they are derived from recombinant sources. Classical genetics will then have to be re-invented and improved. Food additives that are derived chemically may not be accepted easily either. Therefore the focus will be the enzymatic production and liberation of nutrients. New enzymes will be discovered. New feedstocks from the agro sector will be used and consumer needs will change, requiring new conversion technologies. Lower prices will be a continuous goal in this sector.

Overview of high-priority goals

The high-priority goals as defined in the “Vision & Goals” workshop in the Food & Feed sector are:

a. Food challenges:

- **High-priority goal 1: Improvement of functional properties of food.**
- **High-priority goal 2: Production of functional food additives.**

b. High-priority goal 3: Increasing the nutritional value of food. ‘Digestibility’, ‘Processibility / Formulating’ of products are important issues in this context.

c. High-priority goal 4: One-pot modification (hydrolysis (of agro-products) as well as synthesis). Better ‘Cost efficiency’ and less ‘environmental impact’ are important issues here.

High-priority Goal 1: Improvement of functional properties of food

Generally, consumers of food make higher demands compared to the situation years ago. In earlier days the nutritional value of food was the most important property, whereas now properties such as, safety, taste, health aspects, environmental issues, easiness of preparation, variety have become more and more important. Understanding the relation between food properties and molecular structures is necessary to be able to introduce and/or improve the required properties.

Enzymes are believed to play the most important role in achieving the goal. The addition of enzymes has to be divided into improving processing on the one hand and real food additives on the other. Goal is to influence the molecular structure, thereby introducing the required properties. Thirdly, enzymes can be used in processes in which food is produced.

The catalysis toolbox (enzyme toolbox) is (too) small in the Food & Feed sector. There is a relation with the second high-priority goal in this sector which is “production of functional food additives”. In goal 1 enzymes or enzymatic processes have the most important impact on the goal, whereas in goal 2 molecules derived from the fine-chemical industry are believed to have the highest impact on the goal.

It is important to prioritise the required properties of food (environment, health, storage capabilities, third-world issues, etc.).

Goal related development routes are:

- **Novel food additives (enzymes)**
- **New enzymes for food processing**
- **Alternatives for meat of non-animal origin (plants, fungi)**
- **Safe foods**

Technological needs related to these development routes are:

- **Taste and texture expert system:** understanding the functional properties of food and food ingredients. One must be able to understand what is needed on a molecular level to be able to identify and select target molecules and reactions. In an expert system a suitable class of enzymes can be selected quickly. Knowledge about various properties is required, for instance the relation between physical properties of food, such as viscosity, mouth feel and the molecular structure, but also the relation of health related properties, such as allergies. The following scheme visualises what is needed: Functional properties → Molecular Knowledge → Molecules, Reactions → Enzymes
- **Analysis technology:** analytical systems will have to be developed to measure the desired reaction in complex matrices.
- **Enzyme technology:** screening for catalysts for desired reactions: utilisation of known enzymes, discovery and design of (novel) biocatalysts (bioinformatics, directed evolution) for food and feed applications. Additionally: bioprocess engineering and enzyme engineering.
- **Classical genetics technology:** this classical approach will have to be further developed in case the public acceptance of GMOs remains low.

Technologies in “Improved functional properties of food”			
1. Novel enzymatic food additives	2. New enzymes for food processing	3. Alternatives for meat on non-animal basis	4. Safe foods
Catalyst Design & Discovery			
- Taste and texture expert system	- Taste and texture expert system		
- Enzyme technology	- Enzyme technology		
Catalyst Production			
		- Classical genetics technology	- Classical genetics technology
Process Design			
			- Detection systems for microbial and fungal contaminations
Process engineering			
Process Monitoring & Control			
- Analysis technology	- Analysis technology		

Table III.5: Technological focus of catalysis in improved functional properties of food

It may be important to prioritise functional properties on the basis of “higher goals” (for example environment, food safety, third-world issues, etc.).

High-priority Goal 2: Development and production of functional food additives

Consumers are becoming increasingly aware of the influence food has on health and the effect of good or bad eating habits in the long run. By adding bioactive components to food, the food has specific physiological benefits that discriminate them from traditional foods. The additives may help to prevent (chronic) diseases and to enhance the well-being of individuals. In addition, the growing demand for food that contains less salt, sugar or conservatives results in a higher microbiological risk. Food storage and safety will continue to play an important role. In goal 1 the emphasis is enzymes. In goal 2 the emphasis is on chemical molecules as prepared in the fine-chemical industry.

Goal related development routes are:

- **Safety additives (anti-microbials)**
- **Nutraceuticals**
- **Low calorie additives (fat replacers)**
- **Prolonged storage (anti-oxidants)**

Technological needs related to these development routes are fast screening of catalysts and reactions. The primary step will be to develop a toolbox for classification and screening of catalysts for specific properties.

Three different steps are foreseen, which will be tackled in parallel. As soon as new catalysts become available, they should be tested and added to the library. In this way, a better toolbox is continuously built up and knowledge is increased.

- **Analysis system:** A system is required in which chemical compounds can be tested for their effect on specific food properties. Relatively simple in vitro tests should be developed to identify the effect of chemicals on health and safety properties.
- **Development of toolbox:** A toolbox consisting of chemical compounds must be available for screening in the analysis system. This toolbox should come from the fine-chemical industry.
- **Validation of toolbox & possibly building up of expert systems**

Technologies in “Development and production of functional food additives”			
1. Safety additives	2. Nutraceuticals	3. Low calorie additives	4. Prolonged storage additives
Catalyst Design & Discovery			
- Enzyme technology	- Catalyst screening	- (Bio)catalysis toolbox	
- Analysis system			
Catalyst Production			
Process Design			
- Process concept			
Process engineering			
Process Monitoring & Control			
			- Analysis technology

Table III.6: Technological focus of catalysis in development and production of functional food additives

High-priority Goal 3: Increasing the nutritional value of feed

Increasing the nutritional value of feed. “Digestibility”, “Processibility / Formulating” of product are important issues in this context. This is easier than Goal 1, because a lesser (molecular) understanding is necessary. Therefore this seems realistic on the shorter term. Decreasing the need of “animal-testing” may be a “side-issue” in this context; in-vitro tests replacing in vivo tests.

Goal related development routes are:

- **Additives that increase the digestibility of feed** (analogous to phytase)
- **Additives that increase the processibility of feed** (mixing)
- **Catalysis toolbox for Food and Feed** (not detailed in development route graph)

Technological needs related to these development routes are:

- **Rapid, in vitro testing system for digestibility** of feed as an alternative to animal models.
- **Enzyme technology:** screening for catalysts that catalyse reactions that liberate compounds of nutritional value from feed stocks (known enzymes, as well as discovery and design of (novel) biocatalysts using e.g. bioinformatics and directed evolution technologies). Bioprocess engineering, enzyme engineering and directed evolution play an important role here again.
- **Classical genetics technology:** this classical approach will have to be further developed in case the public acceptance of GMOs remains low.

Technologies in “Increasing the nutritional value of feed”		
1. Additives that influence the digestibility of feeds	2. Additives that increase the processibility of feeds	3. Catalysis toolbox
Catalyst Design & Discovery		
- Enzyme technology	- Enzyme technology	- Enzyme technology
- Analysis method	- Analysis method	- Genomics
Catalyst Production		
- Classical genetics technology	- Classical genetics technology	
Process Design		
	- Analysis applications: In vitro testing	
Process engineering		
Process Monitoring & Control		

Table III.7: Technological focus of catalysis in increasing the nutritional value of feed

High-priority Goal 4: One-pot modification

One-pot modification (hydrolysis (of agro-products) as well as synthesis). Better ‘Cost efficiency’ and less ‘environmental impact’ are important issues here. There will be a need for compartmentation, comparable with the ‘FC’ sector. Enzymes and other catalysts for that matter should be compatible in terms of reaction conditions such as temperature, pH, solvent use, etc.

Goal related development routes are:

- **Single reactor processes for starch processing**
- **Novel processes for sugar refining (multi-catalyst)**
- **Continuous food production**

Technological needs related to these development routes are:

- **Enzyme technology:** screening for compatible catalysts that perform the desired reactions at common reaction conditions and that can be used in single reactor systems. Utilisation of known enzymes, discovery and design of (novel) biocatalysts (bio-informatics, directed evolution) as well as bioprocess engineering, enzyme engineering.
- **Process technology:** new multi-step reactors with compartments that contain different catalysts (homogenous, heterogeneous and biocatalysts)

Technologies in “One-pot modification”		
1. Single reactor processes for processing	2. Novel processes (sugar refining, multi-catalyst)	3. Continuous food production
Catalyst Design & Discovery		
- Catalyst screening	- Catalyst screening	
Catalyst Production		
- Enzyme production		
Process Design		
	- Alternative process design	- Alternative process design
Process engineering		
-	- Bio-process engineering	- Reaction kinetics
Process Monitoring & Control		
-	-	

Table III.8: Technological focus of catalysis in one-pot modification

6. FUTURE CO-OPERATION

Introduction

The roadmap as described in the previous chapters provides a framework for future Catalysis related R&D. It focuses on R&D-challenges for the next 10 years and provides high-priority goals, development routes and technologies needed to address these challenges based on a cluster approach. However, the structure and organisation in which the presented challenges are addressed are equally important.

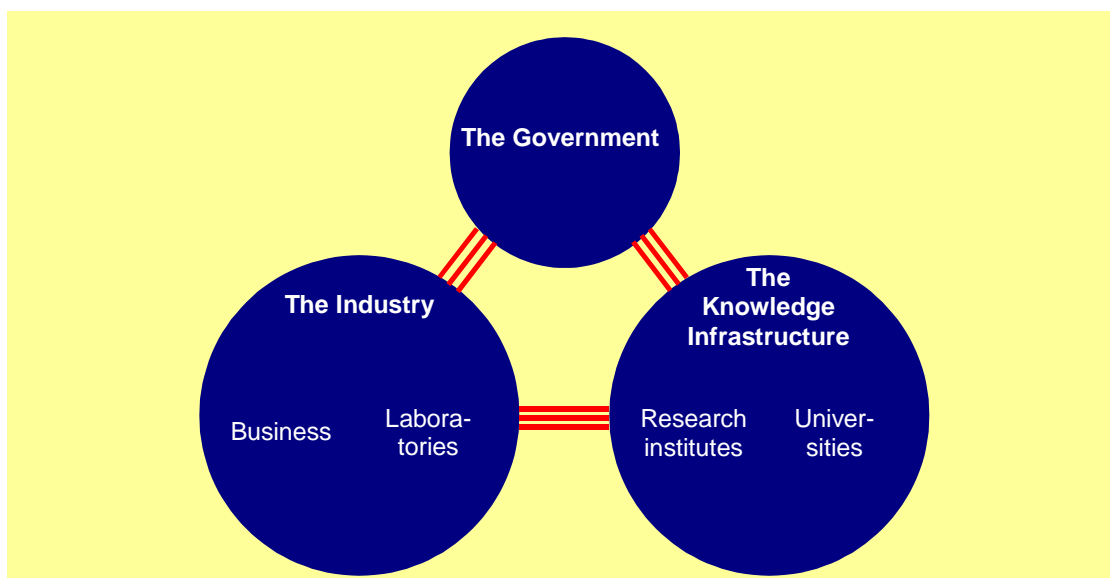
As a result future co-operation within The Netherlands has been a major topic of discussions during the development of this roadmap. This chapter covers the framework used in these discussions and provide a summary of their results.

Discussion Framework

The discussions have been based on involvement of the generic **key-players** in the field and a **co-operation framework** as described below.

Key players involved

In the discussions on future co-operation ‘Industry’, ‘Knowledge Infrastructure’ (universities and research institutes) and ‘The Government’ are distinguished as the key players.



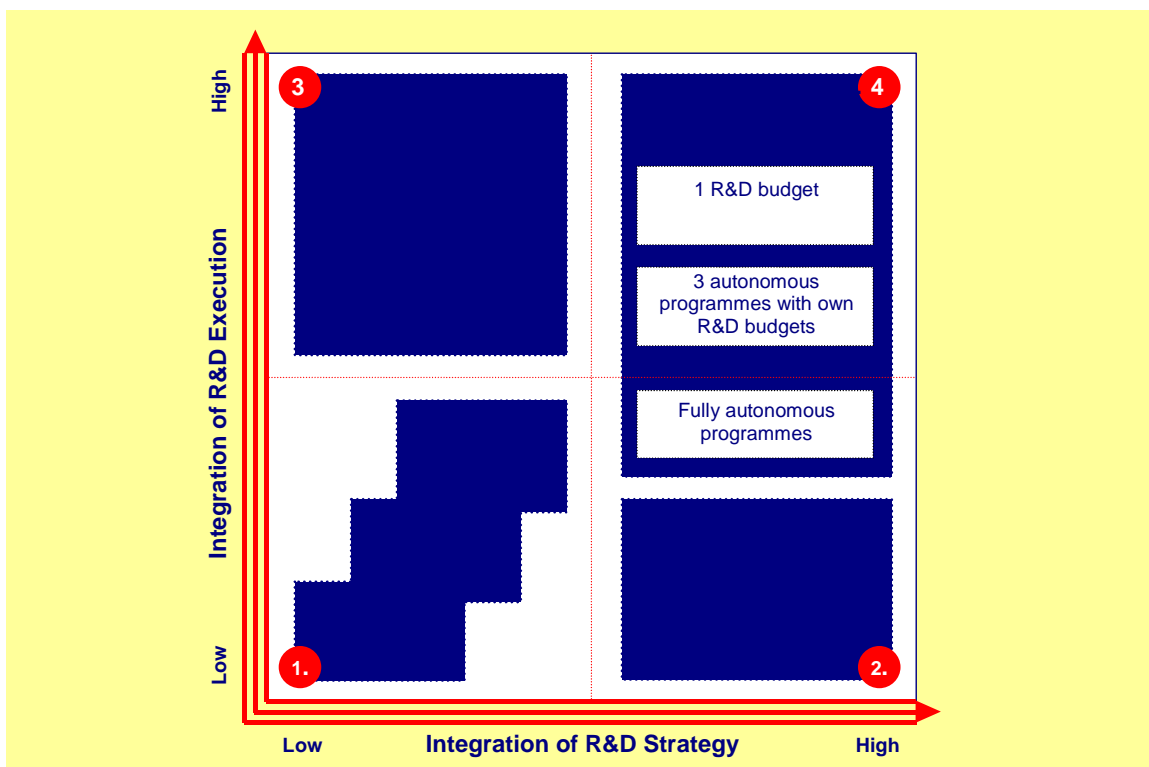
Picture 6.1: Key players in co-operation

- a. **The Government:** Relevant to the Government and its views on co-operation are aspects such as execution of international agreements (e.g. Kyoto), knowledge development and building networks, development of the international position of The Netherlands, technology policy development, legislation, generating interest among new students for the technical disciplines, economic spill-over effects, fulfilling infrastructural needs, etc.

- b. The industry:** The industries view on R&D and co-operation is strongly influenced by aspects such as continuity, profit and shareholder value. Closely linked to this are technological knowledge, image in the society, attractiveness for employees, innovation, etc. In the industry, the trend of research laboratories moving towards the knowledge infrastructure as they are performing more contract research is combined with a strong business focus of research resulting in short-term applied R&D.
- c. Knowledge infrastructure:** Relevant distinction in the knowledge infrastructure is:
- The research organisations/institutes, such as TNO, ECN, etc., perform (contract) research which is relatively close and often directly linked to the industry needs.
 - The universities focus more on long-term fundamental R&D. Education (number and quality of students), scientific excellence (improved scientific profile serves as basis for NWO financing), articles and references and societal goals are important.

Co-operation Framework

In order to structure the discussions on options for future co-operation in catalysis, a framework has been used which comprises of four main concepts for co-operation based on two dimensions. The framework is depicted in picture 6.2.



Picture 6.2: Framework of co-operation concepts

Framework Dimensions

The format covering possible concepts for future co-operation is based on two dimensions, being:

- a. Integration of R&D strategy:** The level of integration of Catalysis R&D strategies of all relevant organisations in the field by means of communications, setting of joint R&D priorities and goals, sharing of information, etc. In high integration, the goals and specific focus of catalysis R&D-activities are collectively determined by a common entity. In low integration each organisation defines its own R&D strategy without any strategic alignment of their R&D portfolios with others.
- b. Integration of R&D execution:** The level of integration in the execution of Catalysis R&D of all organisations in the field by means of joint funding of projects, joint research, sharing of R&D facilities, personnel and equipment, etc. In high integration all relevant organisations and areas (e.g. homogeneous, heterogeneous and bio-catalysis, process and reactor design/engineering, etc.) are included in the execution of catalysis R&D. In low integration each organisation fulfils its own R&D needs.

Four main concepts

This discussion framework results in four main concepts of co-operation. These are:

- Option 1. Individual and (ad-hoc) co-operation:** Characterised by absence of broad formal integration of both R&D strategy and R&D execution in the field of catalysis. Projects can be individual, which may include ad hoc outsourced contract research, or based on (ad-hoc) co-operation within projects. The latter ranges from bi-lateral to cluster projects with a increasing degree of integration.
- Option 2. Taskforce and Catalysis Forum:** Characterised by the development of a joint R&D strategy through development of a vision on the future of Catalysis knowledge and application by a Taskforce (group of recognised experts). Optionally, this could be combined with a periodic Catalysis Forum Meeting in which the organisations in the field discuss and set joint R&D priorities and targets. Implementation of the joint R&D strategy is not organised by the Taskforce but remains the responsibility of the individual organisations themselves.
- Option 3. Catalysis R&D organisation:** Characterised by setting up a joint R&D organisation aimed at providing Contract Research Services (facilities, qualified workforce, etc.) in catalysis. However, without a more focussed collective R&D strategy. Technological working fields are defined by the projects submitted by the partners and other external R&D research contracts.
- Option 4. Catalysis Institute:** Characterised by both a broad integration of R&D strategy in the field of Dutch Catalysis and having joint funds, facilities, workforce for execution of R&D projects. Implementation can range from one overall R&D budget at the Institute level to fully autonomous programmes which fulfil their own budgetary needs. The shape of such an institute can range from “bricks and mortar” to fully virtual.

Discussion Results

The results presented below are a synthesis of the discussions and insights of the three workshops and the final work-conference. They serve as background and starting point for the continued³ discussions and actions related to enhancing catalysis related R&D-collaboration in The Netherlands.

Co-operation needed to address the Roadmap Challenges

The Roadmap Challenges require collective R&D-efforts

The roadmap presents too many challenges which are often too comprehensive to be effectively tackled by individual organisations. The synergy and quantity of the combined R&D-efforts of many organisations in catalysis is needed to reach the roadmap goals.

Chain-of-Knowledge requires involvement of all key-players

The discussions on implementation of the Catalysis Roadmap showed that it should involve all of the key-players. Each of the key-players has specific capabilities in terms of scientific and technological knowledge, R&D-capabilities and facilities, resources, market access, etc. as well as interests. Collectively these capabilities form a chain-of-knowledge reaching from the fundamental development of knowledge to fulfilling market needs which is a prerequisite to achieve many of the roadmap goals.

Structured co-operation is needed in collective R&D-efforts

Each of the involved organisations has specific R&D-capabilities, needs and priorities. In collective R&D, partners have to be found which collectively possess the knowledge and capabilities needed to address the challenges. In addition, an effective and mutually acceptable framework for co-operation has to be established in order to manage the collective efforts and optimise the collective results. The challenges presented in this technology roadmap therefore need to be addressed together with the structure and organisation of the R&D-collaboration.

Integration of both R&D strategy and R&D execution is preferred option for future co-operation

Key-players strive to enhance co-operation in Catalysis

At the work-conference of 7 June 2001 representatives of each of the key-players (Ministry of Economic Affairs, NIOK and VIRAN) presented their view on future co-operation within The Netherlands. All expected added value of enhanced collective co-operation in the field of catalysis and proved committed to further investigate the possibilities for further integration of both R&D strategy and R&D execution.

³ The work-conference of 7 June 2001 was concluded with the collective aim to further investigate the possibility and details of new concepts for co-operation. At that point the Sounding Board of the Technology Roadmap Catalysis was given the assignment to organise these further discussions and investigations.

Collective preference for option 4 (catalysis institute) of the framework

All participants of the final work-conference were asked the question “What should co-operation within catalysis in the Netherlands look like in a few years?”. Results were:

- A strong majority of the workshop participants expressed a clear preference for the upper-right quadrant of the framework (option 4 – catalysis institute) and wanted to further integrate both R&D-strategy and R&D execution;
- Many participants expressed strong objections to integration of just R&D-strategy based on installation of a task-force and/or a periodic conference (option 2 in the framework);
- Integration of just R&D-strategy (option 3 in the framework) is not considered to be specifically undesirable but did not have a clear preference either;
- The few participants voting for the lower-left quadrant showed a preference for an approach based on large cluster projects (of which several examples were mentioned). Main reasons mentioned were that it has more flexibility as not all organisations would need to join the initiative. In addition, many participants stated that this could be incorporated in an overall structure for catalysis and would be a good starting-point towards option 4 (catalysis institute).

Continued discussions should focus on collective benefits and key-issues

Collective agreement to continue discussion on future co-operation

Although the development of Technology Roadmap Catalysis has been finalised with the completion of this report, the discussions on a new structure for future co-operation (addressing the roadmap challenges) continue. The work-conference of 7 June 2001 was concluded with the collective aim to further investigate the possibility and details of option 4. At that point the Sounding Board of the Technology Roadmap Catalysis was given the assignment to organise these continued discussions and investigations.

The collective benefits are the basis for future co-operation

The discussions during the workshops and final work-conference showed that a new form of co-operation within catalysis should be based on:

- **Pre-competitive R&D** as many (mostly industrial) organisations are not willing to engage in a broad collective co-operation when the R&D may directly affect their core-capabilities or core business. In addition, restrictions resulting from anti-competition legislation have impact;
- **Synergy and inspiration in R&D** such as increased speed of R&D, sharing of expertise and people results in better ideas, innovation through integration, etc.;
- **Improvement of the chain-of-knowledge** (from fundamental science development to industrial implementation) through better integration of knowledge development, R&D and application, improved tailor made solutions, alignment of industrial and university efforts, etc. with a focus on (high-risk) pre-competitive R&D;
- **Sharing of R&D costs and risks** such as execution of large, costly and high-risk projects which are not possible or feasible in individual efforts, parallel development of several alternative solutions to a problem, sharing of expensive R&D equipment and joint availability of expertise to use it, etc.

Key-issues need to be resolved

In order to realise a new structure for co-operation which enables collective integration of both R&D strategy and R&D execution in The Netherlands several issues need to be resolved. Key-issue pertaining to co-operation is finding a mutually acceptable solution to the strongly interrelated topics of **funding, resource allocation (R&D focus)** and **IPR**.

- **Funding:** Co-operation in R&D execution requires collective funding. The contribution (size and type) of individual organisations is a major issue in the discussions. General view is that individual funding should be in line with the benefits which are derived from the joint R&D. Establishment of a basis for both funding (e.g. value of knowledge, researchers, use of equipment, etc.) and benefits (e.g. short-term and long-term benefits in different markets, etc.) proved a difficult topic but needs a collective solution;
- **Resource allocation:** The issue of how the collective resources are allocated to R&D-projects is an important issue. Many organisations want to have control over the resources in order to ensure that the research is aligned with their specific needs and interests. A mutually acceptable form of collective control over resources needs to be established;
- **Intellectual Property:** The collective R&D will result in both new knowledge (science and technology) and opportunities to apply it to new and improved product and processes. The issue of access to and ownership of the Intellectual Property (IP) are closely related to the (commercial) exploitation of the collective results. The basis of who has access and ownership of the IP must be clear from the start. A majority of both industry and university participants stated that Universities should not actively strive towards building and exploiting an IP portfolio but should share in the profits generated based on the collective R&D-results.

ANNEX

Workshop participants

The following persons (titles and initials have not been checked for correctness) contributed to this Technology Roadmap Catalysis:

- ir. P.T. Alderliesten ECN, Energie Efficiency in de Industrie
- ir. M. Arninkhof PricewaterhouseCoopers
- Dr. P.H. Berben Engelhard De Meern B.V.
- Prof. Dr. ir. A. Blik Univ. Amsterdam, Instituut voor Technische Scheikunde
- Blom TNO MEP
- R. Bokhorst Ministerie van OC&W
- Dr T.A.B.M. Bolsman NIOK
- Dr. J.A.M. de Bont TNO-MEP
- Drs. N.H.C.M. Boots NOW-Technologiestichting STW
- P. van den Brink Avantium Technologies
- Dr. F. van den Brink DSM Research
- Dr. P.M. op den Brouw Ministerie van Economische Zaken
- Prof. Dr. A. Bruggink DSM Research
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- Dr. U. Dingerdissen Aventis Research & Technologie GmbH
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- ir. H.S. Feenstra Akzo Nobel Chemicals B.V.
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- ing. M.M. Hogendoorn-Wassenaar Norit Nederland B.V.
- A. Hooimeijer Kenniscentrum Papier en Karton
- Dr. M.J.G. Janssen ExxonMobil Chemical Europe
- Prof. Dr. D.B. Janssen Rijksuniversiteit Groningen / GBB
- Prof. Dr. ir. K.P. de Jong Univ. Utrecht, Katalyse Centrum Utrecht
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- Drs. M. Kerkhoffs NOVEM, EET
- Dr. ir. A.P.G. Kieboom DSM-Gist B.V.
- Prof. A.W. Kleyn Universiteit Leiden
- J.H. Koegler ABB Corporate Research
- Dr. Ir. W.T. Koetsier Synetix
- Ing. A. Kok Novem
- Prof. Dr. G. van Koten Univ. Utrecht, Organische Chemie
- Dr. E.G.M. Kuijpers Engelhard De Meern B.V.
- P.W. Kwant Shell International B.V.
- Prof. Dr. N.C.M. Laane DSM-Gist B.V. / Univ. Wageningen
- Prof. Dr. P.W.N.M. van Leeuwen Univ. Amsterdam, Instituut voor moleculaire chemie
- Prof. Dr. ir. L. Lefferts Univ. Twente, katalytische Processen en Materialen
- Prof. Dr. P.J. Lemstra Dutch Polymer Institute
- Dr. D. Liebman DOW Benelux
- Dr. C.M. Lok Synetix
- Dr. A.W. van der Made Shell International Chemicals
- Dr. ir. A.B. van der Meer Akzo Nobel Chemicals / Research
- Dr. R. Meijer KEMA
- Dr. G. Meima DOW Benelux
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- Prof. Dr. ir. W.J. Mortier Exxon Mobil Chemical Europe
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- Volstar TNO
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- Prof. Dr. J.G. de Vries DSM Research

- Ir. W.F. de Vries NOVEM
- K. Vrieze Kon. Ac. Van Wetenschappen
- Dr. W. van der Wal GasTec
- H. van Wechem Shell Research & Technologie Centrum
- Prof. B.M. Weckhuysen Univ. Utrecht, Katalyse Centrum Utrecht
- Dr. A.J.A. van der Weerd Quest International
- Dr. T. Wigmans Kisuma Chemicals
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Technology Classification

The technology classification as developed during the TRM Catalysis process consists of three main technology categories with each several technology fields. The main technology categories are:

- a. Catalysis Technologies
- b. Process and Reactor Technologies
- c. Scientific Methodologies

Catalysis Technologies	
Technology field	Examples
<p>Bio feedstock technology: Catalytic and related technologies for using renewable feeds, ranging from simple derivatisation or functionalisation to full break down into basic building blocks.</p>	<p>biomass gasification renewables conversion cellulose hydrolysis</p>
<p>C1 chemistry: Catalytic and related technologies for the production and use of synthesis gas</p>	<p>natural gas (remote, flare reduction) coal gasification gas-to-liquid</p>
<p>Catalyst synthesis technology: Specific technologies for use in catalyst manufacturing, relating to all reaction components (active species, carrier, media, atmosphere, packaging etc), aiming to improve the properties or increase the catalyst performance</p>	<p>active/selective phase carrier materials</p>
<p>Electrocatalytic module technology: Catalytic and related technologies for building and operation of small modules in which chemicals are directly converted into electricity</p>	<p>conducting polymers fuel cell electrode design electrocatalysis</p>
<p>Hydrogen based technology: Catalytic and related technologies for generation, storage and use of hydrogen as energy carrier</p>	<p>H₂ ad/desorption H₂ manufacturing solar energy conversion small scale H-production</p>
<p>Waste treatment technology: Catalytic and related technologies for (near) in-line removal of waste by-products, for reuse after disposal/end-of-life and for clean-up of pollution/spills</p>	<p>cleaning of waste water/stack gasses soil remediation recycling</p>
<p>Alternative synthesis technologies: "Other" catalytic and related technologies focusing on a specific chemical or conversion methods</p>	<p>current base chemicals (H₂O₂, phenol, PO etc.) selective base chemical production (e.g. cracking/refining: on-purpose alfa-olefin production) CO₂ conversion sensing by chemical amplification polymerisation oxidation (selective O₂ activation) photon catalysed conversion alkane activation anti-Markovnikov olefin hydrogenation</p>

Process & Reactor technologies	
Technology field	Examples
Catalytic engineering technology: Process engineering technologies for specific catalytic conversions, related needs or aspects as well as combinations thereof	multi-step biocatalysis cofactor regeneration fermentation (notably non-sugar feedstocks) immobilisation prevention of deactivation separation (catalytic distillation, supercritical extraction, catalytic extraction, membrane technology, in situ recovery etc.) specific dosing
Novel reactor concepts: Developments in reactor design of importance to catalytic processes	small scale catalysis modules microplant integration of reactor and catalyst design
Novel process concepts: Developments in process design and application of importance to catalytic conversions	closed loop combination intensification miniaturisation modularization simplification
New process media: Developments in process media of importance to catalytic conversions	ionic liquids supercritical fluids
Alternative reaction energy sources: Developments in energy input of importance to catalytic conversions	ultrasound microwave

Scientific methodologies	
Technology field	Examples
Analysis hardware: Specific equipment related technologies of importance to the screening of catalyst functionality	sensors lab/plant-on-a-chip robotics
Analysis applications: Methodologies and technologies of importance to the rapid or specific screening of catalyst functionality	kinetic parameters surface science in situ time resolved spectroscopy (specially resolved anal.) HTA nanoscale analysis
Optimisation tools & methods: Technologies for the rapid generation of options/samples to cover a large parameter space, deterministic as well as via successive selection steps	HTE combiChem directed evolution
Bio-specific methodologies: Combined optimisation tools & methods / analysis applications for the design of biocatalysts, ranging from basic to complex	metabolic engineering genomics proteomics metabolomics
Supportive technologies & science: Chemical and/or physical technologies and themes of importance to the design or (rapid) screening of catalysts	thermodynamics material technology nanotechnology synthesis techniques supramolecular chemistry
Supportive information technology: Information technology related developments of importance to catalyst design and screening	specific IT: modelling (notably computational fluid dynamics) specific IT: bioinformatics general IT: algorithms, datamining
Interdisciplinary science integration: Boundary crossing use of technologies for catalyst design, screening or application	cross fertilisation (bio -> chemo, chemo -> bio)

