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TNO-rapport

0100299532

Meerjarenprogramma 2015-2018 Topsector Chemie Bijstelling 2017

Datum	29 september 2016
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Regievoerend Department	Ministerie EZ
Financierend Deparment	Ministerie EZ
Aantal pagina's	14 (incl. bijlagen)

Summary

In 2016 the TNO Demand Driven Program Sustainable Chemical Industry became more focused after consultation with stakeholders. The program is based on two pillars being Green Chemistry and Smart Materials. Sustainability and functionality is key. Application driven research in Public Private Partnerships with clear targets and ambition form the core of the program. The Public Private Partnerships Biorizon (program on bio-aromatics) and Brightlands Material Center (with the program lines opto electronic materials and lightweight automotive) are regionally embedded respectively in Bergen op Zoom and Geleen. Electrification of the chemical industry is an important topic and is covered in the activities within VoltaChem.

Contents

1 Introduction

The chemical sector is an important supplier of raw materials for many other value chains. An important driver in most of these value chains is to improve the sustainability of products and processes involved. At the end of 2015 the climate conference in Paris again pointed out the importance of CO_2 reduction within the coming years. Within the chemical value chain companies will continue to look for ways to reduce CO_2 emissions in their production processes. Partly this can be reached by using renewable feedstock or renewable energy. In other cases the chemical value chain will continue to develop products that will provide a reduction of CO_2 emissions during their use phase. This can be either by its functionality or because it can be used for example in applications were weight reduction will save energy such as automotive.

Besides the reduction of CO_2 also the security of supply is an important driver for the chemical industry. In some cases alternative feedstock can be a solution to obtain this goal This feedstock can be either from a different source such as renewable materials or obtained via a different production method which is more cost effective. Different production methods for feedstock should provide the possibility to create flexibility. The use of renewables such as biomass are continuously being explored by the industry and the interest in recycled materials is growing. Ultimately the market is interested to use CO_2 as feedstock for the chemical value chain.

In 2015 and 2016 the large chemical clusters in the Netherlands investigated the needs and opportunities to stay competitive. Besides closing loops and making connections between companies, and in some cases with cities, the use of waste heat and waste streams as feedstock for other companies and the opportunities of electrification of the chemical value chain becomes recognized. It is to be expected that renewable electricity will become abundantly available at very competitive prices in the future. This will open up a lot of new opportunities for companies to meet several goals regarding competitiveness as well as sustainability.

In 2015 a new strategy period for TNO started. Within this strategy also a new program for the Topsector Chemie was defined. Each year the program will be adjusted taking into account the actual external and internal developments. On the basis of the Roadmaps of the TKI of the Topsector Chemie, the interactions we had with customers and stakeholders, the previously described trends related to CO_2 and based on the strengths of TNO the program has been adjusted. Due to reduced and more limited financial resources for 2016 and 2017 the program has become more focused. This report describes the annual plan for 2017 and the adjustments to the original program as defined in 2015 and described in the TNO report 0100173227.

2 TNO Program Sustainable Chemical Industry

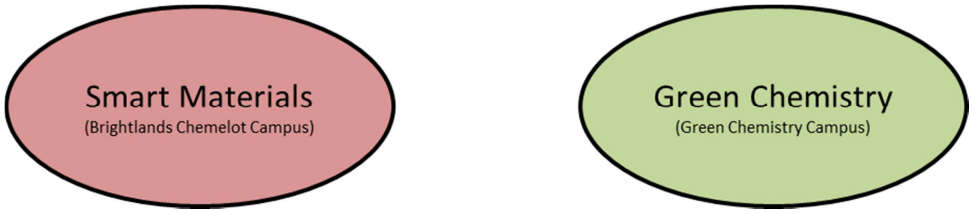
2.1 TNO Program

The original objective of the TNO program for Topsector Chemie was expressed in desired impact achieved at the end of the strategy period (2018). Four different targets were included:

- Accelerating chemical product development: enabling the industry to serve smaller, niche, markets.
- Increasing scalability of production technology: cost factors (n^a) should approach a=1.
- Providing a sound basis for innovation decision taking: a common view within industry and society on sustainability.
- Proven economically viable chemical building blocks from renewable resources (CO_2 and biomass).

Further focusing in 2016 resulted in abandonment of the second impact target and concentration of the activities in three subprograms: advanced materials with the right functionality (AMRF), advanced materials from renewable sources (AMRS), modular and flexible production technology (MFPT).

During 2016, through discussions with industry, TKI Chemie and other stakeholders, the TNO program for Topsector Chemie became even more focused. As a consequence, the third impact target has been abandoned as well and the activities are clustered in two subprograms: smart materials and green chemistry (see figure below).



Higher level goal
Through these two subprograms TNO will contribute to a sustainable chemical industry that enables a sustainable society. We will design and develop together with the industry materials and chemicals of which intrinsic properties offer a benefit for an improved sustainability in the use phase and wherever possible sustainably produced from renewable or recyclable materials like biomass, CO_2 or waste.

The impact of TNO's activities should ultimately lead to implementation on a commercial scale by the industry. Scaling up of the technologies is essential and will be done together with the industry. Public Private Partnerships with a clear focus and challenging applications will provide the ideal setting for the industry to innovate together with other stakeholders in the value chain. These PPPs will play an important role in the overall TNO program for the Chemical Industry.

Subprograms
The subprogram on Smart Materials is embedded in the regional context of the Brightlands Chemelot Campus in Geleen, while the subprogram on Green Chemistry is linked to the ecosystem around the Green Chemistry Campus in Bergen op Zoom. TNO's competencies and activities on innovation decision support

tools (e.g. LCA, ToxRisk, TEA) and process technologies (e.g. print-drying, process intensification, crystallization) are supporting the two subprograms Smart Materials and Green Chemistry.

The TNO activities in these two subprograms are consolidated in three different PPPs: Biorizon and VoltaChem for Green Chemistry and Brightlands Materials Centre (BMC) for Smart Materials.

These subprograms and PPPs are entirely based on the Roadmaps of the TKI Chemie, provided in 2015. The link between the TNO activities and the four Roadmaps of TKI Chemie is described in the table below. Here, colors are used to indicate the extent to which the TNO activities are related to the so called lines within these four Roadmaps. It can be concluded that the current activities of the TNO program are focused on two Roadmaps: Chemistry of advanced materials (Smart Materials) and Chemical conversion, process technology and synthesis (Green Chemistry). The last column of this table (grey) summarizes the TNO competencies in innovation decision support tools and process technologies.

Legend: large contribution, average contribution, small contribution, no contribution.

ROADMAP / LINE		SMART MATERIALS	GREEN CHEMISTRY	TOOLS & TECHNOLOGIES
Chemistry of advanced materials	Designing materials with the right functionality			4, 7
	Thin films and coatings	2, 3		
	Materials for sustainability	7		9
Chemistry of life	Molecular entities, devices and approaches for understanding monitoring and improving personalized health			
	Molecular entities, technologies and approaches for understanding, monitoring and improving food			
	Enabling technologies and approaches for fundamental understanding, monitoring and improving molecular entities in Chemistry of life			
Chemical conversion, process technology and synthesis	Making molecules efficiently			6, 8
	Making molecules from biomass		1	9
	Making functional molecules			7
Chemical nanotechnology and devices	Well-being			
	Cradle to cradle 2.0	5		
	Energy efficiency and storage			

TKI Toeslag projects and proposals:

1. Waste2Aromatics: Conversion of Biogenic Waste into Furanic Precursors for Aromatics
2. *Computational Modelling for Rational Design of Siccatives
3. *Development of Self-Healing Polymer Coatings
4. *Print Drying of Suspensions
5. *Chemical and Mechanical Recycling of Plastics
6. Continuous Complex Nitrations Feasibility
7. *Model Supported Development of Continuous Particle Formulation Technologies
8. *Multiphase Flow for Hazardous Chemistry
9. *Sustainable Chemical Product Performance

The numbers in the table above indicate the first project proposals for “TKI Toeslag” that have an approved fit within the TKI Roadmaps and which is an example of the improved cooperation between the Topsector TKI and TNO. Projects with an * are under development, the other projects are currently (2016) running. It can clearly be observed that most of these projects have a direct fit with the existing TNO activities in Smart Materials and Green Chemistry.

Project #5 seems out-of-scope, but the opposite is true. Within the PPP BMC six program lines were initially defined. Three were put on-hold to quick-start the PPP in a focused manner. One of those three program lines put on-hold has to do with recycling. Project #5 is an exploration of the potential of this program line.

It is anticipated that in 2017 new TKI Toeslag projects will be formulated together with TKI Chemie. The projects should accommodate the needs of the industry as expressed in the TKI Roadmaps, build on the strengths of TNO in certain technology areas as well as to create more focus and critical mass in the three PPPs. Specific topics that could be developed and meet the above criteria are described in chapters 2.2 and 2.3.

2.2 Subprogram Green Chemistry

Objectives for the subprogram Green Chemistry are described below. The activities in this subprogram are carried out in the framework of two PPPs: Biorizon and VoltaChem.

Biorizon is focused on the development of technologies and value chains to convert biomass into aromatic compounds and applications, while VoltaChem strives to develop concepts and technologies for the electrification of the chemical industry.

Biorizon - Objectives & deliverables 2017
Biorizon is a Shared Research Center based at the Green Chemistry Campus in Bergen op Zoom. It is operated by TNO and VITO, while ECN, TNO and VITO signed a letter of intent regarding collaboration of ECN in Biorizon as a leading RTO. Biorizon is focused on new biobased routes to aromatic compounds. The R&D agenda consist of three horizons (program lines): Sugars to aromatics, Lignin to aromatics and a thermochemical route to BTX. TNO is the leader of the sugar to aromatics Horizon and will run a number of projects together with partners from industry. In this Horizon, TNO collaborates with WUR-FBR and Avantium. The following large projects, that are in some cases financed from the VP Sustainable Chemical Industry, were started in 2016 and will still run in 2017. The following objectives for these running projects are foreseen.

Waste2Aromatics: objective for this project is to get a proof of concept for the conversion of biomass into furans. Furthermore a basic design of a pilot plant should be established. Collaboration with waste processors (like Orgaworld, AEB Amsterdam, Twence, Knowaste), water treatment companies (STOWA, Waternet), SABIC (representing the chemical industry).

BIO-HArT: build a skid in the 1-10 kg scale for Diels Alder chemistry to provide a route to functionalized aromatics. Collaboration with WUR-FBR and Avantium, providing technology and samples to Covestro, Klueber Lubricants and Beckers.

Scelio4B: developing a reactor design that will be able to produce suitable dienes (suitable for the Diels-Alder reaction). Collaboration with WUR-FBR and Avantium.

The Province of Noord-Brabant decided on September 23rd to reserve 5 M€ revolving funding for Biorizon, based upon a solid R&D agenda for the next 4 years. It is the ambition to establish a program financing structure, with multiyear commitment from regional and international industrial partners, to accelerate this R&D agenda and consequently the transition to a biobased economy.

Within the realm of TKI Toeslag, an additional project is foreseen like the current project FIAD with industrial partners based on their specific applications (focused on bulk aromatics like Terephthalic acid or Phenol). It is anticipated that in this project a new type of Diels-Alder technology can be further developed, enabling atom-efficient production of bulk aromatics through the use of ethylene and oxygenated/oxidized furans.

Furthermore it is the ambition to establish and extend cooperation's with Universities such as Utrecht but also to seek for cooperation with CBBC or other PPPs.

VoltaChem - Objectives & deliverables 2017

In 2015 VoltaChem has been set up successfully based on TKI transitiemiddelen (2 M€ for a 2-year collaborative project by TNO and ECN) and the Early Research Program (ERP) of TNO on Energy Conversion & Storage. VoltaChem initiates and facilitates collaborative development of technology and business models with relevant stakeholders to help move innovation in the field of electrification and decarbonization faster towards commercial implementation. VoltaChem addresses both the indirect and direct use of electricity within the chemical industry, and works from a systemic point of view. The applied research carried out has made a promising start in the availability of technologies using sustainable electricity to upgrade low-value heat, to increase the efficiency of hydrogen production and to convert chemicals from biomass to feedstock for renewable plastics. Significant steps have been made in 2016, expressed in showcases that are related to hydrogen peroxide, FDCA from HMF and CO_2 conversion. The R&D agenda for 2017 is to continue the research work and to obtain proof of concept through the laboratory demonstration phase.

To enable the full R&D agenda to be conducted, additional financing is required. Therefore, VoltaChem will expand the Community and start new (industry funded) projects. Finally, VoltaChem will explore different options for embedment in an industrial ecosystem (like Geleen, Rotterdam, Delfzijl, etc.).

In 2017, the above mentioned showcases will be further developed into generic toolboxes. The main activities in 2017 will focus on:

- CO_2 (centralized bulk chemicals): together with UU, RUL and UT, improved catalytic systems will be developed to convert CO_2 to ethylene. This will be supported by NWO. TNO will focus on reactor and system development.
- Oxygenate production: based on the FDCA showcase, it has been shown that cost effective renewable hydrogen can be coproduced. Systems will be developed to utilize this hydrogen for the production of oxygenates from CO_2 (DME etc.).
- Electrochemical engineering scale up research, focused on electrochemical oxidation/reduction of biomass.
- Scouting: identification of routes for electrochemically produced small scale ammonia (energy storage and conversion).

Other running projects that will continue:
Also in the domain of Green Chemistry is for instance the EU-FP7 project BIO-QED on the demonstration of industrial biotechnology for the production of building blocks. The 2017 objective of this project is to demonstrate at pilot and demo-scale the best processes for the production of itaconic acid and butanediol. Application research will be carried out during 2017 to find the most suitable commercial application for these two compounds.

2.3 Subprogram Smart Materials

Objectives for the subprogram Smart Materials are described below. The activities in this subprogram are carried out in the framework of the Brightlands Materials Center (BMC), on the Brightlands Chemelot Campus in Geleen.

Objectives and deliverables Brightlands Material Center 2017
BMC consists of multiple program lines, supported by various Demand Driven Programs (VP's). VP Sustainable Chemical Industry is focused on the program lines *"Opto-Electronics"* and *"Lightweight Automotive*".

"Opto-Electronics"
Within the program line *Opto-Electronics* the focus is on development of materials that can be used to regulate the influx by sunlight (other than PV) in the building envelop. Sunlight can be a source of wanted or unwanted heat depending on the time of the day or year. Optical materials can regulate the amount of sunlight that is transmitted through transparent materials or regulate the amount of energy adsorbed by non-transparent materials. The ultimate goal is to make these materials adaptive in order to control the amount of energy passing through. For example warmth should be reflected on a hot summer day (that prevents extra cooling) but in winter could be used to save energy for heating.

These materials can either be coatings or polymer films. Often these coatings and films contain nano-materials in order to provide a nanostructure that will be able to regulate the refractive index. Two large projects will run during 2017 that will provide nanomaterials and coatings containing it.

CO-PILOT
By the end of 2017 a pilot facility will be realized for the production of nanocomposite coatings on kg scale. This facility will also be part of an international infrastructure that offers its services in the field of pilot fabrication of polymer nanocomposites and nanocomposite coatings for other parties in Europe. This pilot production is an important stepping stone for the expansion of such economic activity.

Interreg EnEf
By the end of 2017 a pilot facility will be realized to deposit switchable nano composite coatings on glass and construction panels with the size of 30*30 cm. The optical coatings will provide a better energy performance of the building envelop due to the fact that they provide switchable heat reflection properties.

New projects to be developed within the Opto-Electronics program line.
During 2017 it is the ambition to develop projects that result in for example coatings with anti-fogging properties, wet chemical single layer coatings and optical films providing better heat reflection properties.

"Lightweight Automotive"
Within the program line *Lightweight Automotive* the focus is on the performance of thermoplastic composites for automotive applications. There are several advantages for the automotive industry to use thermoplastic composites because they are contributing to lightweight vehicles, flexibility in design and recyclability. In this way sustainability in the use phase will be improved. Better analysis and predictive modeling of the performance of plastic or plastic containing parts in use, solutions can be found for improvements, but also better predictions of failure can be made.

OP-Zuid project "Proeftuin Thermoplastische Composieten"
Main purpose of the project is to create a demand driven, open innovation platform that offers facilities for design, prototyping, and testing of thermoplastic composites, for a group of Small- and Medium Sized companies in the value chain.
TNO will also supply the following specific expertise's:

- model simulations of mechanical properties;
- in-depth knowledge on adhesion phenomena in TPC's (adhesion between fibre and matrix materials, between layers and between composite and surrounding matrix).

Within the ecosystem in Geleen the automotive application is an important sector.

2.4 TNO competence on Tools & Technologies

Objectives for the supporting tools and technologies are linked to running projects in this field. These projects are directly or indirectly linked to the programs on Smart Materials and Green Chemistry, but are set up in such a way that the developments and results strengthen the overall competence portfolio of tools and technologies. Illustrative is the planned participation in an EU project on LCA methodology development. Although the targeted user case is not directly linked to either BMC, Biorizon or VoltaChem, the resulting knowledge improves our LCA capabilities and contributes as such to the total proposition of the TNO program for chemical industry.

Two examples of running projects and their deliverables for 2017 are given below.

EU-ToxRisk will drive a paradigm shift in toxicology towards an animal-free, mechanism-based integrated approach to chemical safety assessment, uniting all relevant disciplines and stakeholders to establish pragmatic, solid read-across procedures incorporating mechanistic and toxicokinetic knowledge, and *ab initio* hazard and risk assessment strategies of chemicals with little background information. The expertise developed in this project connects to the Diamonds platform reported in "Voortgangsrapportage VP Chemie 2015". It enables industry to select the most promising new or alternative products in an early development stage. As such, it connects to the three PPPs BMC, Biorizon and VoltaChem where biobased chemicals or new materials are targeted. During 2017, the EU-ToxRisk project will apply the toolbox developed in 2016 to (industrial) cases for validation.

The Sustainable Chemical Product Performance project (initiated with DSM, Covestro and Solvay) led to the identification of best practices and gaps for application of sustainability assessment in the area of Sustainable Portfolio Management. Based on the identified gaps, a follow-up was formulated in which Covestro and Solvay will most probably join (this follow-up is in the form of a TKI Toeslag project, #9). The objectives in 2017 are to develop and test new

approaches to improve on white spots in current sustainable product portfolio management methods, being the use phase, time perspective and product LCA segmentation. The following results are anticipated: 1) a pragmatic, robust and validated approach for taking into account the sustainability impacts of the use phase of consumer end-products in Strategic Portfolio Management, 2) a scenario approach to include time sensitivities and scenarios in the sustainability assessment of both production and consumer end-products and 3) a scientifically underpinned guideline for segmentation of LCAs of products and proxies to estimate impacts of new products. These results are not only relevant for these companies, but can be used by a broader spectrum of organizations. The developed methods will also be used for the execution of BMC, Biorizon and VoltaChem.

3 Dynamics

In the interaction with stakeholders and industry it has been recognized that a focused TNO program for the chemical industry based a select number of application driven research topics will ultimately result in a knowledge base that supports the industry in the most optimal manner. The need for sustainability and improving the competitiveness of the Dutch industry are key drivers for TNO's program. Green Chemistry and Smart Materials are enabling these drivers.

Application driven research with a clear Roadmap towards commercial implementation by the industry provides the guideline to develop technologies that are internationally outstanding. The development of excellent knowledge will support the Dutch chemical sector in the international field. The way to obtain this, is by focused Public Private Partnerships with clear Roadmaps towards implementation. In 2016 further emphasis has been put on strengthening the three PPPs Biorizon, VoltaChem and Brightlands Materials Center.

Within these PPPs TNO will further seek in 2017 the collaboration with the industrial value chain in the relevant ecosystem but also with universities and other knowledge institutes.

For Biorizon
- Strengthening collaboration by involvement of ECN
- Installing new program financing structure and governance
- Increased interaction with industry across the value chain

For Voltachem
- Link to regional ecosystem
- Strengthening knowledge on selective oxidations
- Acquire additional funding and building industrial consortia

For Brightlands Material Center
- Cooperation within the local ecosystem but also with universities and "Hogeschool" by supporting PhD's and providing lectors
- Building up unique infrastructure but also provide access for industrial partners through collaborations
- Building up competence on modeling

4 Signature

Eindhoven, September 29th, 2016 TNO

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