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TNO report

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Contents

1 Introduction

TNO launched its new strategy in 2015 and with it the new programmes for the Topsectors for the period 2015 – 2018. The Demand Driven Programme (VP) Sustainable Chemical Industry is among those programmes. This report describes the annual plan for this programme in 2016 and gives an outlook for the further development of the programme in the coming years. The document describes mainly the changes compared to the original plan as described in TNO report 0100173227. Although this text is written to be as self-contained as possible, it may be useful to refer to the original plan for more background information.

The year 2015 turned out to be eventful and crucial to the Topsector Chemical Industry. Three important developments have a profound impact on the TNO programme:

1. The newly founded “TKI Chemie” and the “TKI BBE” developed new roadmaps for the sector[1,2]. They provide a firm, new, foundation for the programme that was unavailable when the programme started in 2015.
2. In the new innovation contract (2016 and 2017), TNO has to accommodate a large budget cut. In previous budget cuts, the chemical sector has been spared. Now, the available budget will be reduced by approximately 50% from 2016 onwards. This inevitably means the ambitions of the programme must be altered.
3. One of the goals for 2015 was the formation of a “core” for the different programme lines. This has been achieved by setting up strong cooperation with two regions: the Brightlands Materials Centre in Southern Limburg and Biorizon in Western Brabant and Zeeland. These two cores provide a sound long-term foundation for the programme with strong infrastructure, regional support and industrial commitment.

This report starts with an overview of the broader activities of TNO and the relevance for the chemical sector. Subsequently it focuses on one of the programmes: the Sustainable Chemical Industry Programme. Chapter 2 provides an overview of the programme and its ambitions and the link to the roadmaps of the Topsector. The programme consists of three lines. These lines are discussed in Chapters 3 – 5. Each of these chapters starts with a brief description of the line. Then an overview of already ongoing projects is given. The plan for 2016 is described in terms of new projects to be developed and started in 2016, thus filling gaps in the programme and progressing towards the ambition of the programme for 2018.
The development of the programme consists of developing projects in Public Private Partnership. The overall portfolio of projects should, when executed properly, lead to achieving the goals of the programme. This development is governed by the programme councils and strategy board of the Topsector Chemie. However, the project development and execution is done within the knowledge organisation, TNO in particular. How this process to develop the programme is governed is described in Appendix 1.

[1] KIA chemie (in Dutch) http://Topsectorchemie.nl/uploads/userfiles/Roadmaps%20Topsector%20Chemie%202016-2019%20DEF.pdf (link may change in October 2015)
[2] Research agenda Biobased Economy 2015 – 2027 (in Dutch) http://edepot.wur.nl/338385

2 TNO and the Topsector Chemie

2.1 The chemical sector is about connections, so is TNO

The chemical sector is, in many cases at the root of the industrial value chain. Innovation in the chemical leads to new materials and opportunities for innovation in sectors downstream in the value chain. Historically, most activities of TNO for the chemical industry were inspired from TNO activities in other sectors. It is therefore useful to evaluate the Sustainable Chemical Industry Programme within the context of the other ongoing programmes for industrial sector in the chemical industry value chain. The sustainable chemical industry is, at it were, supplementing many other activities at TNO relevant for the sector with some activities that are really specific to the chemical sector.
The TNO programmes, excluding the activities for defence and security are listed in Table 1.The most relevant programmes for the chemical sector are highlighted in that table. This document describes just one programme: sustainable chemical industry, but it is important to remember that this programme is executed in an environment where much more relevant knowledge and research is being executed.

Innovation in the chemical sector is always the result of a collaboration with other sectors. In the Brightlands Materials Centre, the connection between the chemical and the high tech industry leads to new, functional, materials. TNO's contribution to the Brightlands Materials Centre consists in part of the programme line "advanced materials with the right functionality" in the Sustainable Chemical Industry Programme. The other part is the programme line "additive manufacturing" in the Programme Flexible and Freeform Products and part of the programme 3D manufacturing instruments.

On the Green Chemistry Campus, the connection between the chemical industry and the agrofood sector leads to the development of chemicals and materials from biomass. TNO's contribution to this endeavour is mainly contained in the programme line "advanced materials from renewable resources", but the programmes geo-energy, sustainability and environment and food and nutrition are important too.

The connection between the sectors energy and chemical industry lead to many new possibilities such as CO_2 conversion and electrochemistry. The Sustainable Chemical Industry Programme is making that connection in the programme line "flexible and modular production technology", but the programmes sustainable energy, complexity and energy conversion are relevant as well.

Currently, the Programme Sustainable Chemical Industry does not yet connect to the life science sector. This connection does offer many potential advantages, for example as a source of inspiration for new chemicals and materials from biomass. The connection between chemical industry and life sciences is made in the programmes personalized food and health, making sense of big data and predictive health technologies.

This report describes the content of the Sustainable Chemical Industry Programme. The other programmes are described in similar reports.

Table 1 Overview of TNO sector related programmes excluding the defence and security related ones

Theme	*Programme*	*Topsector(s)*	*Societal topic*
Industry	Flexible and Freeform Products	HTSM	
	Space and Scientific Instrumentation	HTSM	
	Semiconductor Equipment	HTSM	
	Networked Information	HTSM	
	Sustainable Chemical Industry	Chemie	
Healthy Living	Predictive Health Technologies	Life Science	Healthcare (Min. VWS)
	Food and Nutrition	Agrofood	
	Prevention Work and Health		Labour (Min. SZW)
Urbanisation	Mobility and Logistics	Logistiek	
	Environment and Sustainability		Environment (Min. I&M)
	Buildings and Infrastructures		Environment (Min. (I&M and Min. BZK)
	Smart Cities	Water	
Energy	Sustainable Energy	Energie	Energy (Min. EZ)
	Geo-energy	Energie	Energy (Min. EZ)
	Maritime and Offshore	Water	Offshore Energy (Min. EZ)
Cross-sector early research programmes	Quantum Computing and Quantum Internet	HTSM, Creatief	
	Complexity	Life Science, Chemie, Logistiek, HTSM, Energie	
	Personalized Food for Health	Agrofood, Life Science	Min. VWS
	Energy Storage and Conversion	Energie, Chemie, HTSM	Min. EZ
	3D Nanomanufacturing	HTSM, Chemie,	
	Instruments	Life Science	
	Structural Integrity	HTSM, Chemie	Min. I&M
	Human Enhancement	Life Science	Min. VWS
	Making Sense of Big Data	All	Min. EZ

2.2 Three programme lines to connect the Topsector roadmaps

The programme as described in the original plan contained six programme lines. The reduction in government funding to TNO has resulted in a reduction of the funding available to the Sustainable Chemical Industry Programme with 50%. Such a reduction can only be achieved if the scope of the programme is also reduced considerably.
At the same time, the roadmaps of the newly formed TKI Chemie have become available. These roadmaps are interdependent. They are structured according to knowledge area or technology and they need to be combined for many applications.

Applied research and development is therefore almost inevitably a combination of the knowledge and goals of two or more roadmaps. The TNO programme should provide the links and cement to combine the roadmaps towards solutions for societal and industry issues.
Both new developments have led us to restructure the programme into a smaller programme with three lines instead of six. These lines were chosen to facilitate cross-overs between the TKI roadmaps (including BBE) and to coincide as much as possible with the two regional agendas of respectively Geleen and Bergen op Zoom. It is the intention to concentrate on these regional agendas. Table 2 lists the new programme lines and provides a mapping of these lines on the regional agendas and the previous structure of the programme.

Table 2 Mapping of the new programme lines on the programme lines of 2015 and on the regional economic development agendas

Line	*Composed of previous lines*	*Description*	*Regional Focus*
Advanced materials with the right functionality	Innovation decision support Electrochemistry development and CO_2 utilization	Development of new functionality in materials through new molecules or formulations	Brightlands, Geleen
Advanced materials from renewable sources	Performance materials from renewable sources Sustainability management	Development of new formulations and molecules for niche applications where renewable sources offers distinct advantages	Green Chemistry Campus, Bergen op Zoom
Modular and flexible production technology	Flow chemistry development Electrochemistry and CO_2 utilization	Development of new processing technologies to enable the production of materials in the other two lines	Brightslands, Geleen and Green Chemistry Campus, Bergen op Zoom
Discontinued	Biomass processing and biorefinery	Activities in this line will be continued in two TNO spin-out companies	n/a

The relationship between these new programme lines and the roadmaps is shown in Table 3. This relationship is not static. For example, the table shows that there is still little connection between the programme and the Chemistry of life roadmap, whereas TNO does have interesting knowledge to contribute to that roadmap. One of the goals for 2016 is to develop additional projects that enhance that connection.

Table 3 Mapping of the programme lines with the roadmaps

ROADMAP / LINE		ADVANCED MATERIALS WITH THE RIGHT FUNCTIONALITY	ADVANCED MATERIALS FROM RENEWABLE RESOURCES	FLEXIBLE AND MODULAR PRODUCTION TECHNOLOGY
Chemistry of advanced materials	Designing materials with the right functionality			
	Thin films and coatings			
	Materials for sustainability			
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			
	Making molecules from biomass			
	Making functional molecules			
Chemical nanotechnology and devices	Well-being			
	Cradle to cradle 2.0			
	Energy efficiency and storage			

2.3 The ambition of the programme

The desired impact of the programme was formulated in 2015 in four goals:

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

In view of the decreased funds available for the programme, this ambition must be reviewed as well. It was decided that goal 2 (scalability of production technology) is no longer an explicit goal of this programme. Hence, there is no connection with the sub-roadmap “making molecules efficiently” anymore. Obviously, some results of the programme will still contribute to scalable production technology, but there will no longer be projects developed for that explicit purpose.

3 Advanced materials with the right functionality

3.1 Programme line goals and focus

This programme line aims to develop new materials that have dynamic or responsive functionality. The materials interact with their environment in such a way that the material itself changes properties in response to changes in the environment.
Initially this is done for niche applications where this type of behaviour offers high added value. It is the vision of this programme line that these new materials will develop from niche applications into large scale, bulk, materials.
The focus of this line is on the Brightlands Materials Centre.
Niches to be addressed are (at this moment):

- **Opto-electronics**: materials to transmit or block light depending on triggers, wavelength specific behaviour.
- **Lightweight automotive**: materials with property gradients, suitable for additive manufacturing. Highly tailored local material properties following design requirements.
- **Energy conversion and storage**: materials that respond to light energy and electrocatalytic materials.
- **Sustainable packaging**: materials that actively promote shelf life or indicate product quality.

3.2 Ongoing projects

This programme line coincides with the recently started Brightlands Material Centre. Most projects therefore are still in the stage of project development and have not yet start. However, two projects are already running.

3.2.1 CO-PILOT

CO-PILOT is an EU Horizon 2020 project with the aim of developing and constructing a pilot line for the production of nanoparticles.
The field of nanocomposites materials has witnessed remarkable progress in recent years with many different types of nanocomposites exhibiting radically enhanced properties for a wide range of industrial applications. In order to enable SMEs to enter this crucial stage of the research-development-innovation cycle, the European Commission has challenged larger enterprises and research and technological organizations to get together in order to provide a coordinated network of pilot lines, test and validation services for SMEs in order to prepare for management decisions to progress to the next step of new technology deployment, i.e. installation of industrial pilot lines and enter the commercialization stage.

The CO-PILOT consortium took this challenge and built a project that intends to develop an open access infrastructure for companies interested in the production of high quality (multi-)functional nano-composites on a pilot scale. The pilot reactor will be able to produce batch sizes of nano-composite polymers and coatings in the range of 20 to 100 kg’s. The development of the pilot plant infrastructure will be achieved by including different types of nano-composites as model systems.

Online-monitoring during the pilot-manufacturing process will allow following the nano-particle dispersion quality.

3.2.2 EUToxRisk

The EUToxRisk project was awarded in 2015 under Horizon2020. The project aims to develop assessment methodologies to assess the health effects, beneficial and detrimental, of new materials in development. The availability of such tools can guide the development of new materials in several ways:

1. It provides early indicators of the possibility to register the new material on the European market.
2. It provides early indicators of the safe usage potential of the materials.
3. It guides the development of new molecules by providing insight in biological activity of new molecules and compounds.

3.3 New projects to be developed in 2016

The current ongoing project provide the basics for material development. In 2016 a number of application oriented projects should be developed and started. Currently the following ideas exist.

1. A project on modelling the chemical activity of siccatives in coatings, with the purpose of developing new drying agents for paint. These new drying agents should replace toxic components and improve drying times and quality.
2. Self-healing coatings. a number of industrial partners expressed interest in developing new self-healing coating concepts.
3. Development of anti-dust coatings.
4. Anti-reflective coatings using nanoparticles with self-organizing properties.
5. Materials for energy efficiency (heat storage).

4 Advanced materials from renewable resources

4.1 Programme line goals and focus

Materials from renewable sources are desirable from the point of view of sustainability. However, in most bulk applications such materials are struggling to compete with more traditional, fossil based, materials. The incumbent production has some inherent advantages. The technology is already optimized and installations are already built and frequently written off.
This programme line focuses on the development of materials from renewable resources (biomass, CO_2) where there is an advantage in the application for renewable materials. Some of these advantages are:

- Functionality that can only be found in “natural” materials.
- Marketing advantages: consumers are sometimes willing to pay a premium for renewable materials.
- Local availability of raw materials, allowing better deployment of the value chain.

The programme line focuses on materials with small world market volumes and high added for markets such as:

- Personal care
- Home care
- Aromatic compounds

This programme line is executed together with the Biobased Delta, on the Green Chemistry Campus.

4.2 Ongoing projects

The past three years, two large projects to produce aromatic compounds from biomass and specifically sugar were started in collaboration between VITO, DLO, TNO and the Green Chemistry Campus. These projects form the core of this programme line. Besides, there is also a development on the sustainability of these materials.

4.2.1 Biorizon

Biorizon is a Shared Research Center with an initial focus on technology development for the production of functionalized biobased aromatics for performance materials, chemicals & coatings. Biorizon is anticipating the expected growing shortage of aromatics from the petrochemical industry and the widely shared ambition to green the chemical industry.

Our goal is to be a leading European Center for functionalized biobased aromatics within 3 years and to be in the global top 3 within 5 years. This way the participating companies will get the best results possible!

Biorizon is a cross-border initiative between TNO, VITO and the Green Chemistry Campus and is part of Biobased Delta. Biorizon is located at the Green Chemistry Campus in Bergen op Zoom, The Netherlands, at the heart of industries between Antwerp and Rotterdam.

Global leaders in the fields of feedstock, conversion, equipment and end products are invited to join our industry driven Shared Research Center that is based on the open innovation methodology.

4.2.1.1 The industry's need for biobased aromatics

Aromatic building blocks represent a very significant share of our today's building blocks, not only in order to create fuel components, base chemicals or polymers, but also to create polymer additives, colorants, flavors and fragrances. Currently virtually all aromatic building blocks are made from fossil oil that will become scarce. Hence, it is important to develop technology to replace the current aromatic petrochemical based building blocks by alternative feedstocks.

Shale gas and shale oil are rapidly emerging as a new feedstock, but will produce mainly light fractions such as ethylene/propylene, and no aromatics in gas-fueled crackers. Given the global challenges that society is facing with respect to CO2 emissions, pollution, global warming and shortage of suitable fossil oil reserves, new biobased production routes need to be realized urgently to address the ecological and economic challenges that humanity and industry are facing.

4.2.1.2 Industry driven Shared Research Center

Setting up a sustainable and economically successful commercial scale business, is a major challenge in this field. A significant research effort is needed, more than one single organization can handle. Therefore Biorizon is operated as a Shared Research Center, based on the open innovation methodology, bringing together collective intelligence of various industries, companies and knowledge organizations. The multi-disciplined technological need, as well as the long term roadmap make this effort suitable for shared research, sharing intelligence, investments, risks and workload.

We aim to include the global leaders in the fields of feedstock, conversion, equipment and end-products as participants in the Center, as well as SME companies.

4.2.1.3 Ambition: global top 3 within 5 years

Our ambition is to be a leading European Center for functionalized biobased aromatics within 3 years and to be in the global top 3 within 5 years. In order to achieve this, we will build up a group of minimum 50 FTE scientists and technologists and grow this team every year, both in size and quality. Resident technologists of the participating companies will work closely together with the core team of VITO and TNO. This will assure the best results for our partners. The results of Biorizon will allow the partners to commercialize biobased business successfully.

4.2.2 AERTOS

The AERTOS consortium unites the seven largest RTOs in Europe in the area of bio-economy. In this consortium Fraunhofer, VTT, Sintef, SP, Tecnalia, VITO and TNO jointly develop basic new technology for the production and use of sugars from lingo-cellulose, the use of aquatic biomass and the use of lignin.
Furthermore the consortium analyses the market of biobased materials and provides a joint insight in the opportunities and barriers for developing materials from renewable resources[3].
Together, the AERTOS have a portfolio of over 100 M€ per year in ongoing research and development on biobased materials and energy.

4.2.3 Sustainable chemical performance

The sustainable chemical performance consortium is an industry consortium that aims to develop an open source, generally accepted, benchmark methodology to assess all aspects of sustainability of a chemical product (molecule, material, formulation). The driver for this development is to enable transparent, open and credible communication with customers and society on the sustainability performance of products from the chemical industry. This should enable more robust decision taking in product development and prevent unforeseen side-effects from new material developments.

4.3 New projects to be developed in 2016

The project portfolio in this programme line is already very mature. The focus in 2016 will be to strengthen these projects with new industrial partners. Also the Biorizon project needs to develop a more long-term perspective together with the Biobased Delta.
In 2016 the knowledge base of this line will also be enhanced by involving additional knowledge institutes in the projects. The AERTOS consortium will be more involved in Biorizon and ECN will be added to the consortium.

[3] See https://insightrefinery.wordpress.com

5 Modular and flexible production technology

5.1 Programme line goals and focus

The advent of new energy and raw material sources, new business models and new (nano)technology necessitates a thorough rethinking of the way chemicals and chemical formulations are produced. The general consensus is that there will be a need for cost efficient small scale and modular production technology in the near future, thus reversing the trend of economy of scale.
Introducing new production technology is difficult in this mature industry, especially in Europe where there is little room for expanding production capacity. It is the philosophy of this programme line, that new production technology needs to be developed primarily to enable the production of new chemicals and formulations. Once the new technology has proven itself in these new application, it may trickle down to existing installations as well.
This programme therefore focuses on supporting the developments in the other two lines with the development of new production technology. It is useful to concentrate these developments in a separate line, because there are many similarities in the development of process technology between the two material development lines.
In terms of technology, the programme line focuses on three technologies:

- Functional nano-materials synthesis
- Encapsulation
- Electrochemistry

5.2 Ongoing projects

5.2.1 Electrification of the chemical industry

The main ongoing project is the electrification project together with ECN. This project is part of the transition plan of the Topsector Chemie. The goal of this project is to develop options for the chemical industry to use electricity as an energy source for the production of chemicals. The main energy source currently is natural gas, whereas most renewable energy sources provide electricity.

TNO also invests in this development through the early research programme “Energy Conversion and Storage”. The two projects are twins and are closely linked.

5.2.2 CyclicCO2R

Besides this project, there is also a project on CO2 as a feedstock for the chemical industry. The objective of CyclicCO2R is to create a process that removes the dependency on fossil fuel and increases the energy efficiency to create a net CO2 uptake in the production of cyclic carbonates, especially glycerol carbonate. As an inexpensive waste product from bio-diesel production, glycerol will be the main raw material, along with CO2, ensuring cost effectiveness and, thereby, a maximum commercial potential. Two production routes will be explored in order of preference.

A direct route: converting glycerol directly to glycerol carbonate. Starting point will be the use of pure glycerol, but ultimately impure glycerol derived directly from

biodiesel production will be used. Main challenges reside in the catalyst activity and the necessity to remove both water and product in-situ.
An indirect route: converting glycerol to glycerol carbonate, through the formation of epoxides. The indirect route has the potential to create enantiomerically pure cyclic carbonates.

The aim of both routes is to use impure CO2 directly from the source. Besides these 2 routes the feasibility of producing the starting materials for the production of cyclic carbonates from CO2 and H2O using sustainable energy will be evaluated resulting in a roadmap for their implementation.

The research will is on:
- Developing the optimal catalyst-process combination in terms of activity, catalyst recoverability and optimal immobilization technique. Make the process capable of using impure glycerol and CO2.
- Intensifying the reactions in a continuous flow reactor, focusing on energy efficiency and increased product yields. Optimize the productivity by in-situ removal of products and by-products.
- Creating a mini-plant scale process which starts with the impure renewable raw materials and CO2 and produces cyclic carbonates.
- Completing the design of a scaled-up process integrated with a chemicals plant so that the developed technology is directly transferrable to industry.
- Provide techno-economic analysis of the process showing the commercial and environmental feasibility of the process.

The CyclicCO2R project will finish in 2016.

5.3 New projects to be developed in 2016

The main focus in 2016 will be on two things:
1. Involving industry as contributing partner in the electrification project.
2. Developing a sequel to CyclicCO2R together with the Green Chemistry Campus and the TKI BBE.

6 Signature

Eindhoven, September 21st, 2015 TNO

A.J.A. Stokking
Managing Director Industry

A Governance of the programme

Hierarchy of programme elements
The programme sets goals and ambitions for a period of four years. For practical reasons the programme is subdivided in programme lines.
The main way to achieve these goals is through the execution of projects. Projects are the activities that are planned and agreed upon with partners. All partners in the programme enter on the project level and they are a partner because they participate in a project.

The task of governing the programme therefore consists of:

1. Setting long-term goals and ambitions
2. Identifying which projects are desirable in order to reach the goals
3. Developing the desired projects by involving partners, applying for subsidy grants etc.

Within TNO, there are two types of projects:

- Projects that require public funding
- Projects completely funded by industry

The latter are not explicitly part of this programme, although they often contribute to the goals of the programmes. They are created at the explicit request of (a consortium of) companies.
The former starts with the availability of public funding (matching) at TNO. In general there are two different sources of public funding that can serve as the seed of a new public-private project development:

1. The government contribution to TNO, SMO (Samenwerkings Middelen Onderzoek)
2. TKI funding

The former is the result of TNO's contribution to the innovation contract. The latter is the result of a supplement on private contributions to developments at TNO. Both are governed through the Topsector Chemie and the TKIs Chemie and BBE.
It was agreed that the two sources will be regarded as one source of public funding and will be governed through one annual governance process with the TKIs. TNO is expected to keep track of two distinct sources and manage project development in such a way that the respective conditions under which these sources may be used are met.

The governance cycle can be summarized as follows.

September:	TNO writes rolling agenda for next four years (this report).
October/November:	Review by TKI and Topsector, resulting in advice to EZ.
December:	EZ grant to TNO for next year based on advice Topsector.
February:	TNO submits report over last year to EZ and Topsector.
March/April:	Review of report by EZ and Topsector.
May:	Outline for new update of rolling four year agenda.
June/August:	Discussions with stakeholders.
September:	TNO writes rolling agenda for next four years.