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Thema Chemie****Industrie**De Rondon 1
5612 AP Eindhoven
Postbus 6235
5600 HE Eindhovenwww.tno.nlT +31 88 866 50 00
F +31 88 866 88 19

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Auteur(s)	Ir. P.M. Wolfs, Dr. ir. Jan Harm Urbanus
Autorisatie	A.J.A. Stokking Managing Director Industry
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1 VP Sustainable Chemical Industry

1.1 Introduction

This report describes the results achieved in the first year (2015) of the TNO program for the chemical industry for the period 2015-2018. The ambition and related objectives of this TNO program are described in TNO report 0100173227. The ambition of this program is expressed in the desired impact of the program in 2018 and in new competences that TNO must acquire during the program.

The desired impact of the program is:

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).

Since the new TNO program is a continuation of and extension on the previous (first) TNO program for the chemical industry, several activities were already defined and running when the new TNO program started. In addition, new activities were initiated in order to progress toward the four impact goals. The existing and new activities were clustered in six program lines. The year 2015 turned out to be eventful and crucial to the Topsector Chemical Industry. Three important developments have had a profound impact on the program:

1. The newly founded "TKI chemie" and the "TKI BBE" developed new Roadmaps for the sector. They provide a firm, new, foundation for the program that was unavailable when the program 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 program must be altered.
3. One of the goals for 2015 was the formation of a "core" for the different program 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 program with strong infrastructure, regional support and industrial commitment.

These developments have resulted in the reformulation of the ambitions of the TNO program and a restructuring of the activities. In terms of impact goals, the second impact goal has been abandoned. In terms of restructuring of activities, the original six program lines have been replaced by three program lines that hold tight relations to the regional initiatives. The TNO report 0100289197 (Sustainable Chemical Industry Program – Annual plan 2016) describes the relation between the old and new program lines and the four Roadmaps from TKI Chemie. The new structure is used as basis for the reporting of the results of 2015. The three program lines within the new structure are:

- Advanced materials with the right functionality (AMRF)
- Advanced materials from renewable sources (AMRS)
- Modular and flexible production technology (MFPT)

The relation between these program lines and the three impact goals is depicted in the table below.

Program line / Impact goal	Accelerating Chemical Product Development	Innovation Decision Taking	Renewable Chemical Building Blocks
AMRF	XX	X	0
AMRS	X	X	XX
MFPT	X	0	X

1.2 Program 2015

1.2.1 *Advanced materials with the right functionality*

As explained in the description of the four-year TNO program, collaboration between different research and technology organizations, academia, industrial companies and (regional) authorities is very important in the European innovation landscape. It was therefore of utmost importance to establish such 'collaborative cores' for the three program lines TNO is active on. The press release pictured below about the Brightlands Materials Center (BMC) shows that such a core was established for the program line "advanced materials with the right functionality" in Geleen, Limburg.

PRESS RELEASE - Launch of the Brightlands Materials Center

In *Nieuws* On 19 maart 2015

Sittard-Geleen, 19 March 2015 – Today, TNO and the Province of Limburg have opened a new international research and development center to further untap the potential of polymeric materials at Brightlands Chemelot Campus in Sittard-Geleen, The Netherlands. Partners will invest 45 million euros in the new center over a period of five years. The Brightlands Materials Center will bring top scientists and industry professionals together to develop sustainable, breakthrough materials and application technologies that will change the market.

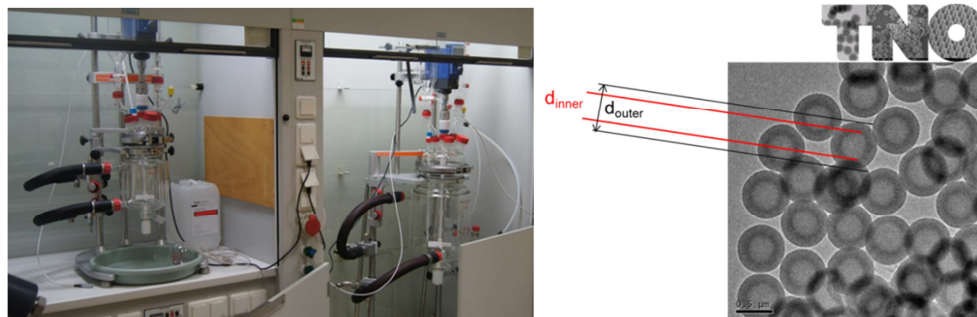
More than 15 organizations have expressed their interest in participating in BMC, resulting in various projects and project proposals that have been developed during 2015. A total of six program lines have been defined, of which three are currently fully operational: Additive Manufacturing, Lightweight Automotive and Opto-Electronics. The TNO program for the chemical industry is primarily sponsoring the program line on Opto-Electronics, while the TNO program for HTSM is focused on Additive Manufacturing. On top of BMC related activities, TNO continues the development of chemical synthesis routes, of materials, of formulation technologies and of innovation decision support tools that jointly contribute to the proposition of "advanced materials with the right functionality".

Highlights of the results in 2015:

CO-PILOT

CO-PILOT is an European (KP7) project and part of the BMC program Opto-Electronics. It is focused on realizing piloting infrastructure for the manufacturing of nanoparticles and nanocomposite materials. This year TNO established infrastructure at 2L and 15L (see picture below) as to accommodate technology transfer up to 100L (at the premises of project partner Fraunhofer). In addition to the

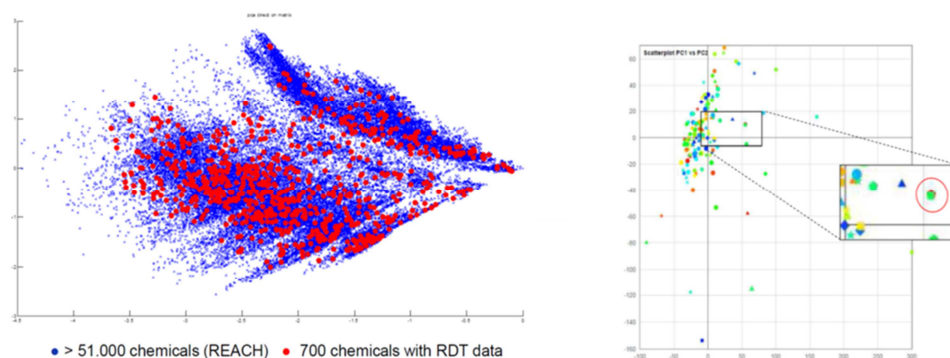
depicted reactor, TNO has implemented analytical instruments to monitor the production process of nanoparticles online.



Furthermore, TNO realized a basic design for downstream processing steps to enable the formulation of nanoparticles into composite materials. Finally, activities for surface modification were initiated last year as well as methods to analyse the quality of the final nanocomposite material. Hence, the basic requirements have been fulfilled to start the production of hollow silica spheres and semiconductor nanoparticles in 2016.

DIAMONDS

During 2015 the development of DIAMONDS tools for safety assessment of chemicals was accelerated. DIAMONDS includes computational chemistry tools and models for predictive toxicology and structure-property relationships. With DIAMONDS new product innovations can be faster, cheaper and more sustainable (for instance requiring less animal testing). In 2015 publicly available pathology and omics (in-vivo and in-vitro) data from various sources was integrated in a workflow with user-friendly dashboards (see pictures below, left: chemical space with Repeated Dose Toxicity data in red versus chemical fingerprint of 51.000 REACH chemicals, right: biological response of in-vitro liver cells for >150 chemicals). With DIAMONDS it is now possible to predict and assess a chemical's toxicological profile, both for designing safer new chemicals, as well as finding alternatives for existing unsafe chemicals.



1.2.2 Advanced materials from renewable sources

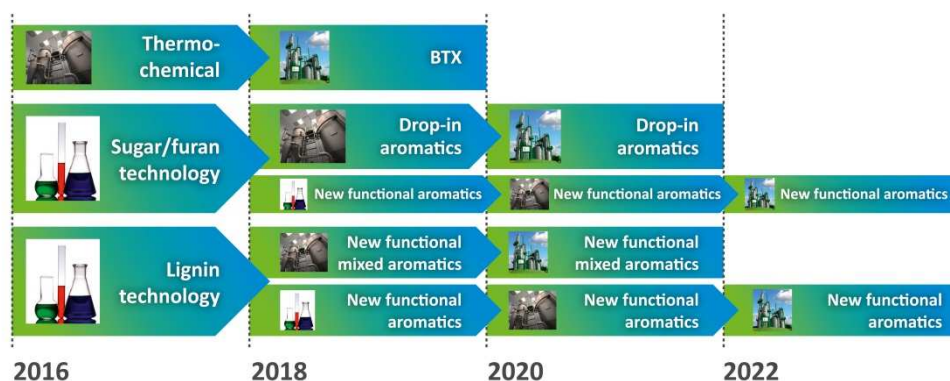
The 'collaborative core' for the TNO activities on renewable sourcing is the Biobased Delta, the region encompassing the provinces of Noord-Brabant, Zeeland and Zuid-Holland. Here, TNO is present at the Green Chemistry Campus through the Shared Research Center Biorizon. In addition to the work related to bio-aromatics, TNO has been developing technology for the whole lignocellulose value chain: bio-refinery technology, fermentative production of organic acids and

valorization of lignin. In addition, TNO developed innovation decision support tooling for the assessment of sustainability and for the mapping of innovation aspects in regions. Altogether, the technologies and tools support the transition toward a Biobased economy.

Highlights of the results in 2015:

Biorizon

Biorizon experienced a very successful 2015 with excellent project results, with interesting project proposals receiving very positive feedback, with commitments from several companies to participate in cash in projects, with the filing of 5 patents and finally with massive publicity on “Waste2Aromatics”. In November the second Biorizon Community event was held, with more than 70 participants from all over Europe. During this meeting an updated Roadmap was presented. This Roadmap (see image below) is the result of numerous conversations and discussions with industry and serves as Biorizons compass toward commercial production of bio-aromatics by 2025.



BioConSepT

In the context of fermentative production of organic acids, TNO was active in two European projects to develop and demonstrate new technologies. One of them, BioConSepT, came to a close in 2015. The final year of this project was focused on piloting of new technologies and value chains. TNO coordinated this project and collaborated with several RTO's and highly interested companies to demonstrate new technology for the production of FDCA, a very interesting chemical that can be used to replace the PET-bottle for a more sustainable alternative. The pictures below show process equipment (crystallizer, filter) and pure crystals obtained with this process.



GAIA

GAIA, “getting algae ingredients applied” is a joint development with the TNO program Food & Nutrition. In 2014, the VALORIE pilot plant for bio-refining of aquatic biomass (like algae) has been established. This year it has been used to retrieve valuable data concerning scale-up. The data has been used for techno-economic evaluations that delivered two major insights: 1) bio-refining of biomass into multiple products is favourable over the production of single-products from aquatic biomass and 2) bio-refining of algae is cheaper than the autotrophic production of algae (autotrophic means using light and CO₂). Finally, VALORIE has been used to produce sufficiently large samples for application testing. It has been shown for instance that algae pigments can be used in coatings.

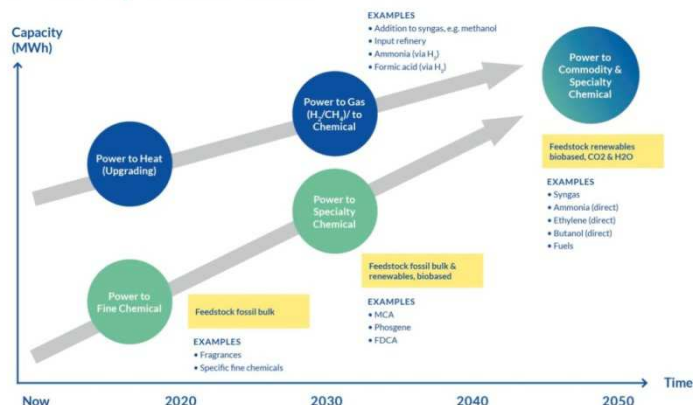
1.2.3 Modular and flexible production technology

This program line is focused on the development of small scale and modular production technology that should facilitate the transition to new energy sources (renewable electricity), new feedstocks (biomass, CO₂), new business models and the increased use of nanotechnology. As such, this programme line is supporting the developments in the previous two programme lines and a separate ‘collaborative core’ is therefore unnecessary. Amongst the technologies relevant for this programme line are multiphase flow processing, electrochemistry, print drying and CO₂-chemistry.

Highlights of the results in 2015:

Electrochemistry

High level Road Map of Electrification



Just before Christmas '14 the collaboration between ECN and TNO on “Electrification of the industry” was initiated. During 2015, this collaboration was launched as VoltaChem during an event with ‘Topsector Chemie’. This collaboration is crucial with regard to the symbiosis of the energy and chemicals sector in the future. The Roadmap of VoltaChem is depicted above. Results for 2015 are reported separately in the paragraph 1.4.

Multiphase Flow Processing

During the last few years an impressive portfolio of Multiphase Flow Processing capabilities has been assembled, which culminated during 2015 in the construction of a flexible, multi-purpose skid at bench-scale (1-10 litre per hour) with which Proof of Concepts for various multiphase flow processes can be demonstrated. This skid-mounted equipment (see picture below) is the link between TNO's expertise and

infrastructure at lab-scale and the pilot-scale facilities at Coriac partners DSM and Janssen Pharma. As such, TNO has acquired the ability to accelerate time-to-market of new developments from industrial partners in this important field.



1.3 Overview cooperations

Overall, collaboration of TNO with other knowledge institutes (RTO's, universities, etc.) and with companies increased significantly. The major example is the kick-off of BMC, which resulted in joint research with a number of companies. Another example is VoltaChem that launched its community through which participation and collaboration of knowledge institutes and companies is promoted. Within Biorizon the link with three waste management companies was established, while furthermore, the link between Biorizon and InSciTe, the research institute located on the Brightlands Chemelot Campus, was reinforced, culminating in a joint research project.

In conclusion it can be stated that the TNO program for the chemical industry is well underway toward achieving the impact goals.

- The initiation of the Brightlands Materials Centre, as well as the advances in the different production technologies have the potential to accelerate the development of new products.
- The development of new business models and new tools, together with industry, for the assessment of sustainability of value chains, economic viability of technology, and of toxicological risks related to innovative products, are laying the foundation for the desired next level in innovation decision taking.
- The ongoing developments in Biorizon and VoltaChem will lead to pilot demonstrations of chemical building blocks from renewable resources (biomass and CO₂) and will as such enable the chemical industry to make the transition to a more sustainable industry.

1.4 TTI Transitie Chemie – Electrification of the Chemical Industry

The transition plan is the first start of a large cooperation program between TNO and ECN ("VoltaChem" - <http://www.voltachem.com/>) on the use of green electricity as energy source in the chemical industry. The implementation of the technology,

models and methods that are developed will enable the industry to make use of more flexible production, in terms of energy, feedstock and product range. Also investment profiles will change, making it easier for the industry to adapt to market changes (compared to a lock-in because of existing CAPEX). For society this means more product diversity and products targeted at specific segments, less energy use, sustainability and more feedstock flexibility. Scientifically, the project will deliver results as demonstration of technologies will show that the science can indeed lead to economic activity.



The focus of the program is on 4 topics:

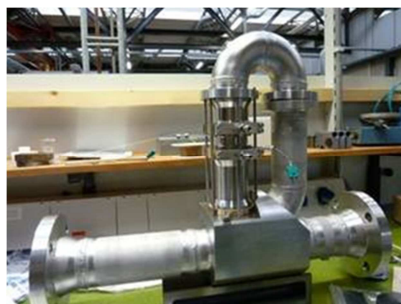
- Community
- Power to Heat (P2H)
- Power to Hydrogen (P2H2)
- Power to Chemicals (P2C)

The activities are aligned with the research done in the Early Research Program, topic Energy Storage and Conversion, Electron to Chemicals (ref. "Annual plan 2015 – TNO ERP 2015").

COMMUNITY - The activities within the community, where ECN and TNO are working closely together, bring together stakeholders from relevant sectors (chemicals, energy, equipment industry and service providers) in an exclusive forum. A multi-year high-level Roadmap for implementation of electrification and decarbonization in the industry and society as a whole is developed and maintained (see figure in main SCI summary). Specific high-level non-technical projects that are needed for implementation of the Roadmap are carried out such as technology-, innovation-, and business scouting, value web analysis for electrification technologies & markets, development of hit-lists for industrial electrification options, development of frameworks for infrastructure integration, development of electrification scenario's and policy and organizing workshops and events. External parties can join the community with an in-cash or in-kind contribution. Six partners have joined the community (Magneto, NUON, Cofely, TNO, ECN, Topsector Chemie). Other parties currently involved are DIFFER, Solliance Eindhoven, JRC, ISPT, Deltalinqs, TU Eindhoven, TU Delft, Dow, Arkema, OCI Nitrogen, Akzo Nobel, Hydrogenics, Stedin, Siemens, Technip, Hydron Energy, Proton Ventures and Innovation Quarter. In November RVO approved a 'SI Project E-Match Hit-list for Electrification'; Matching Processes with Electrification Technologies together with Arkema, Akzo Nobel, OCI Nitrogen, Stedin and Dow. The kick-off meeting has been held in December 2015.

POWER TO HEAT (P2H) - Power to Heat means the use of renewable electricity (e.g. wind, solar and hydro) as source to upgrade heat and steam. This involves the development of high temperature compression heat pumps, a combination with heat and cold storage, and the development of alternative concepts for heat generation & upgrading, e.g. electrical heating, steam compression & multifunctional heat pumps. Work within this topic is done at ECN. A modelling tool

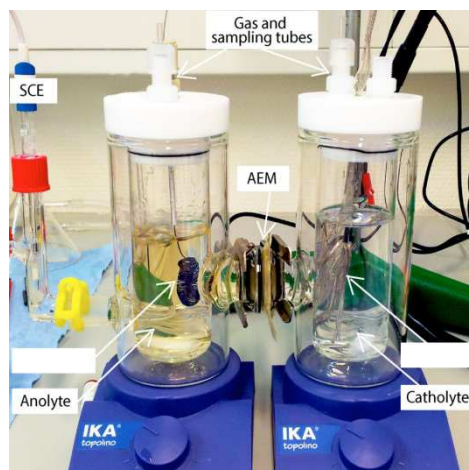
has been developed to assess the performance of several refrigerants (working media) for high-temperature compression heat pump applications. Refrigerants have been evaluated for a delivery temperature of 180°C. Although suitable media have been identified, the thermal stability of these media at the required temperatures seems questionable. In addition, an assessment has been carried out on the type of compressors that should be used for this application. An inventory has been made on commercially available electrically driven heat pump technologies and on compressor suppliers. In addition, new developments have been identified.



Three new electrically driven heat pump concepts have been evaluated. A system study is performed where an 1 MW Multifunctional Thermo-acoustic Conversion Unit system is assessed that is combined with an existing gas engine or gas boiler. The MTCU is build-up of multiple standardized modules. It has been shown that a standardized module can operate both as cooler or heat pump or both combined over wide range of operating temperatures. An analysis has been carried out that shows that the heat pump performs well over a range of temperatures (50 - 150°C), without changing the design. The same system design is also capable of producing electricity from waste heat.

POWER TO HYDROGEN (P2H2) - The main objective of this topic is the use of renewable electricity as energy source for direct chemical transformations via hydrogen, where in P2H2 the focus is on efficient hydrogen production. Work within this topic is executed by ECN. Activities are business case development for flexible industrial H2 production, development of combined electricity storage and H2 production and the development of novel concepts for PEM electrolyzers. In addition, two internal workshop sessions involving experts from different backgrounds have been held with an external moderator. Furthermore, three devices were purchased to test their capacity to generate H2 and to evaluate the electrical power required per kg H2 produced. A small test environment was created for testing these devices in terms of I-V behaviour in relation to hydrogen production. The preliminary conclusion from the first test results is that the business case looks positive. Further development of this technology is discussed with ISPT and TU Delft.

POWER-TO-CHEMICALS (P2C) - The main objective of this topic is to use renewable electricity as energy source for conversion of raw materials to chemicals and fuels, where P2C is focused on the electrochemical conversion of renewable raw materials as feedstock for chemical production. Feedstocks are e.g. biobased feedstock, biogas (CH4), H2O, O2, N2 and CO2. Work within this topic is done at TNO. The Roadmap for P2C has been finalized.



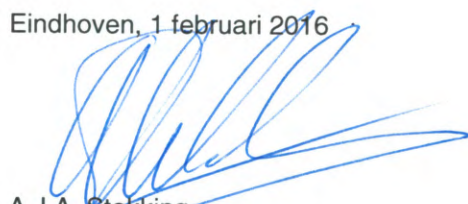
A showcase is developed to demonstrate the possibilities of electrochemical selective oxidation, specifically the conversion of HMF from bio based feedstock to FDCA, a potential building block for renewable plastics. Optimal reaction conditions have been studied based on lab scale conversion experiments. The experiments indicated that the oxidation is favored at pH values higher than pH 12, with increasing pH being more favorable in terms of current density (and hence the oxidation rate of HMF). For the acidic conditions, other electrode materials specific for low pH, as PbO_2 and NaBr were not selective for FDCA production. Based on the results, promising electrode materials, conditions and electrochemical setups have been proposed. Following the 'workflow' approach, the downstream processing for the HMF to FDCA electrochemical oxidation route is developed. A number of process concepts has been designed and analyzed on high level. A ranking of the concepts has been done for application in an integrated process.

IN CONCLUSION - In 2015 a program has been set up successfully to initiate and facilitate 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. The program 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. The goals for the next year are to continue the research work into the laboratory demonstration phase and to expand the VoltaChem program with new collaboration partners and new industry funded projects.

2 Ondertekening

Eindhoven, 1 februari 2016

TNO



A.J.A. Stokking
Managing Director Industry