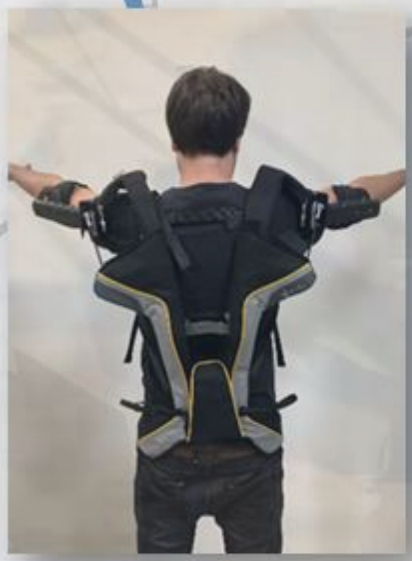
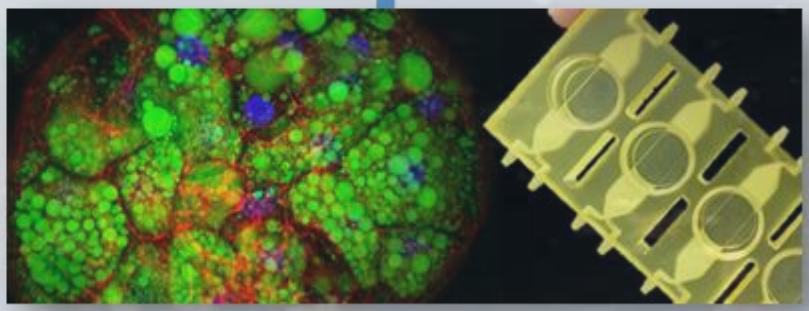
TNO innovation for life

Innovation for life





TNO EARLY RESEARCH PROGRAMS

Annual Report 2020

TNO-report: TNO 2021 R10115

TNO EARLY RESEARCH PROGRAMS
Annual Report 2020

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Contents

1 Introduction

In this report we present the 2020 progress of TNO's Early Research Programs (ERP) portfolio; see the funnel in Figure 1. The plans corresponding to the results reported here were described in 'TNO Early Research Program Annual plan 2020' (reference TNO 2019 R11669, dated October 31st, 2019).

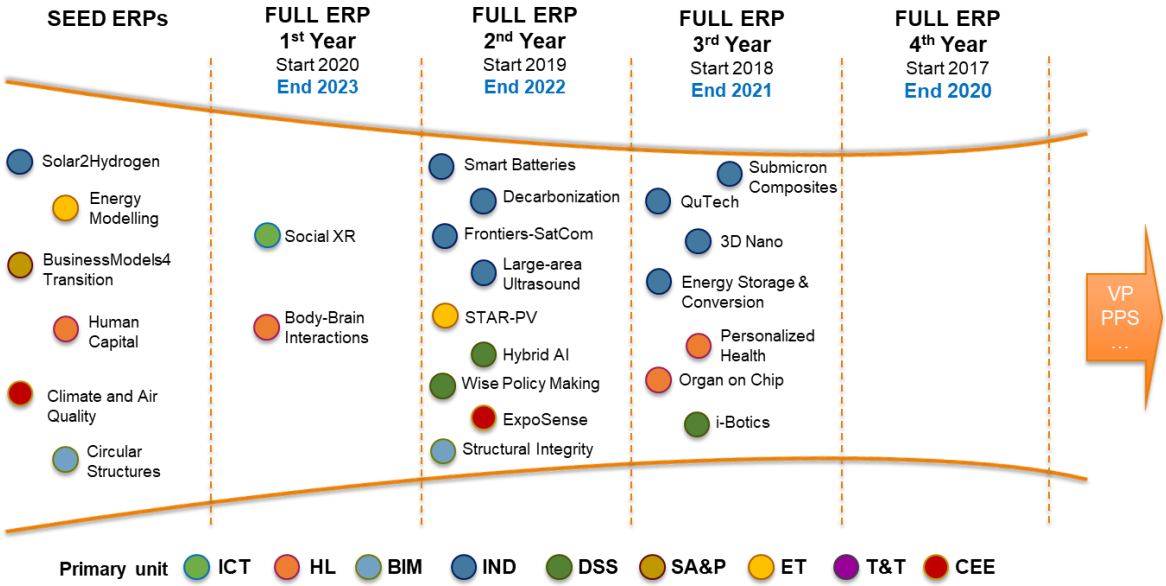

Figure 1 ERP Funnel 2020

In total 18 Full (four-year) ERPs were being carried out (see Table 1), focused on societal and economical grand challenges requiring a concerted effort of fundamental and applied research, to be succeeded by future private development. We continued our use-case-inspired research approach with emphasis on generating *cutting edge knowledge and technology* together with research partners from academia, and on *building research ecosystems* with stakeholders and sponsors from industry and public organizations. Table 1 below lists these ERP's and provides for each of these a (few) 2020 highlight(s).

Table 1: Full ERP's Highlights 2020

Full (four-year) ERP's	
(Link to) Chapter: ERP-title *Short description*	Highlights 2020
4th year projects: Start 2018 – End 2021	
2: **Quantum Computing** *We exploit quantum effects in customized systems, materials and concepts, such as quantum computing and communication to pave the way for a second revolution.*	In April 2020, QuTech launched Europe's first public quantum computing platform: 'Quantum Inspire'. Quantum Inspire makes the quantum computer accessible to everyone. It contains a processor made of highly promising semiconductor 'spin qubits'. The electron spin qubit (with high computation power) is made with the same technique as a classic transistor and is just as small. This makes it suitable for mass production. The platform also provides access to a processor made of superconducting (transmon) qubits – a unique combination. Users can experiment with quantum algorithms and compare the processors.

3: **Energy Storage & Conversion** *Using renewable electricity and sunlight, CO_2 and green H_2 as a feedstock, we produce C1 chemicals and fuels providing a great opportunity to store energy, to overcome the inherent fluctuations in supply of renewable energy and the spatial and temporal mismatch between demand and supply.*	In the electrons-to-chemicals research line (using renewable electricity as energy source to drive chemical reactions) a completely new process concept for electrolysis of CO_2 has been added to the set of concepts under exploration: a concept using an undivided cell. With this 'one compartment electrolysis' feasible formic acid production was demonstrated. The concept led to a patent application. For further development it was included in a Horizon 2020 proposal submitted this year. In the photons-to-chemicals research line (using sunlight as the energy source to drive chemical reactions) strategies for commercially feasible photo(electro)chemical conversion of CO_2 to methanol have been developed. Furthermore, optimized catalysts for the plasmonic photoconversion of CO_2 to methane with respect to activity/space-time-yield were developed, this work has been published. The first design of a complete lab scale mini-factory for the conversion of CO_2 to methane and syngas has been completed, the setup will be delivered in 2021. A Horizon 2020 proposal was submitted and granted this year.
4: **3D Nano Manufacturing** *We create breakthrough solutions for semiconductor metrology for the next generations of chips by developing and exploiting scanning probe microscopy in all its different modalities. Additionally we facilitate innovation in neighbouring areas like bio-technology.*	For the purpose of measuring smallest 3D details in next generations of chips, the further development of Sub-Surface Probe Microscopy has a central role in this ERP. In 2020, our piezo devices at the core of our SSPM concept were demonstrated to have almost the required sensitivity and were consecutively further improved, allowing us to deliver definite proof of feasibility of this technology early in 2021. Furthermore, two new modalities were added to the program: single tip quantum sensing and IR-AFM for chemical identification on nanomaterials.
5: **Personalized Health** *We develop a system providing personalized advice on sustainable lifestyle habits based on biological understanding of inflammatory dynamics, dysmetabolism, AI modeling and health community support.*	With a proof-of-concept mouse study we demonstrated that lifestyle interventions can reverse chronic inflammation and obesity related pathologies. We received medical ethical approval for the human proof of concept study to show that personalization based on the innovative combination of biology, personality and behavior results in a more effective intervention to improve health and that this approach is scalable. A demo was made of the modular Personal Health Advice System, focusing on lifestyle related health. We described the social contract between patients (data donors) and data processors (researchers) that serves as a framework for FAIR usage of personal health data.
6: **Organ Function on Chip** *With an advanced organ-on-a-chip preclinical toolbox we enable the inclusion of human diversity in the preclinical phase of drug development and the selection of the right candidate drugs and right patients for clinical trials.*	We have demonstrated the applicability of our 'organ-on-chip' technology in a number of use cases, enabling the introduction of population variability earlier in drug development. This will enable development of precision medicine, support selection of drug candidates effective for specific group of patients. For example, with our 'InTESTine chip' holding human tissue with microbiota we have shown populational variability in drug absorption and epithelial immune responses to various compounds.

7: **Submicron Composites** *We develop smart, responsive materials by precisely controlling their chemical composition and micro/nanostructure. Examples are nanostructured coatings and nanocomposite polymer films for thermochromic energy efficient windows and 3D-printed fiber reinforced composites with high strength and integrated sensing functionality.*	In 2020, we fully optimized the performance of our single layer thermochromic glass coating on lab scale, and concluded that it outperforms single and multilayer coatings reported in literature. Furthermore, we have successfully developed thermochromic nanoparticles which can be used as pigments in polymer films. In collaboration with Hasselt University, we studied the switching kinetics of thermochromic powders and coatings in detail, and published the results in Solar Energy Materials and Solar Cells. Furthermore, we developed 3D printed fiber-reinforced thermoplastic composites with high strength and integrated sensing functionality. Latter is based on integrated carbon fibers, which can be applied for electronic sensing and structural health monitoring of the respective object.
8: **i-Botics** *We focus on optimal human-robot interaction in challenging, unpredictable, dynamic situations. The focus areas are human controlled robots based on telepresence perception and manipulation capabilities for e.g. installation, maintenance, repair and emergency response; and wearable robots for human enhancement in rehabilitation and heavy work environments.*	We built a demo of a bimanual tele-operated setup augmented with another arm. We continued work on interpreting the VR environment and creating symbolic object representations and their transfer to live operators in a multi-sensory VR environment for situational awareness. A demonstrator of an active back support exoskeleton and a controller optimized for effectiveness and usability in practice were built, including multiple algorithms targeted to generate a real-time estimation of the bending forces in the lower back. We created a sensor-based tool which helps determine the potential for exoskeletons in heavy work.
3rd year projects: Start 2019 - End 2022	
9: **Structural Integrity** *We develop digital twins (simulation models fed with sensor data) mimicking the behaviour of macro-structures and guiding the design and management of these structures. Main challenges are multi-scale modelling, advanced sensing techniques, high speed computing and AI learning capabilities.*	We implemented a demonstrator using our Digital Twin platform involving monitoring and generation of asset management data of the steel bridge use case which we had selected. We matured the distributed fibre optic sensing technology so that it can now be used in the Moerdijk bridge, which will be our living lab in the next years. Artificial Intelligence design models were validated and calibrated of structures for high dynamic loading occurring in blast conditions.
10: **ExpoSense** *We develop solutions for personalized promotion of health based on non-invasive assessment of external and internal exposure profiles to Particular Matter (PM), by developing accurate, reliable and calibrated PM sensors and by predicting and interpreting personal external and internal exposures by quasi real-time modelling*	A particle sensor was designed and constructed that can measure the chemistry of airborne Particulate Matter (PM) in real time (collect > 95% of all PM in air), based on new designs of a mini-cyclone that concentrates airborne particles 2000-5000 times, and in-line infrared spectroscopy. We realized a field test at a construction site showing sensitivities between 500 – 30000 µg/m3 PM and the capability for the chemical identification of crystalline and amorphous silica. During the field test we demonstrated in real time visualization and a first interpretation of the exposure levels for personal feedback to end users on a mobile device through a cloud service.

11: **Future Optical Satellite Communication** *By using laser light instead of radio we aim to greatly enhance communication between satellites, ground stations and airplanes, providing ultra-high data throughput and ultra-secure and multi-point communication.*	In 2020 we developed an improved system concept of a ground communication terminal capable of transmitting data at 10 Terabit/s to a Geostationary Orbit satellite as well as a concept of a high secure key rate optical channel for a Low Earth Orbit-satellite.
12: **Wise Policy Making** *We develop a suite of instruments and methods to support policy makers to assess the impact of policy options on wellbeing (ex-ante) and to engage in unbiased and well-informed dialogue leading to decisions that prioritize sustainable societal wellbeing.*	We developed a prototype of the Wise Cube (a tool to analyse expected impact of alternative policies on wellbeing), including a quantitative model and interactive dashboard. To support the identification and avoidance of biases in policy making, we developed a Neuro-evolutionary Bias Framework that provides insights into the neuro-evolutionary origin and underlying working mechanisms of cognitive biases. This Bias Framework has been published and has been included in the prestigious Encyclopedia of Behavioral Neuroscience.
13: **STAR-PV** *By gaining insight in and by developing improved control of basic degradation mechanisms we enable improved reliability and sustainability and lifetime extension (e.g. beyond 20 years) of integrated thin film devices (photovoltaic and other opto-electronics) integrated in building components and products.*	In this program key progress has been in enlarging our understanding of why panels fail (degradation mechanisms). In 2020 we developed a specific technology to take small samples out of used solar panels ('coring') and to analyse these. With it, a.o. we investigated the mechanism of degradation caused by partial shading of CIGS solar panels.
14: **Large-Area Ultrasound** *We develop technology for large area, flexible ultrasound imaging/monitoring systems enabling to bring medical care to the home environment. Our essential approach is to build printed ultrasound transducers using cost effective display fabrication technologies.*	Large-area ultrasound imagers with multiple imaging 'pixels' will open new approaches and applications in medical imaging. We have optimized a thickness mode transducer which, unlike all other solutions available, is fabricated using an imprint and replication process that can be scaled to large area. The technology merges concepts from thin/thick film processing, display fabrication as well as nano-imprint technology. We have improved the performance of our thin-film transducers and readout by a factor of 4000 since January 2020, now to the actual level required for medical imaging.
15: **Smart Batteries / Self-Adapting Smart Batteries** *Battery packs (e.g. for cars) contain thousands of individual cells, grouped in modules. By introducing sensors at cell or module level, batteries can be controlled more smartly. We develop technologies to enable this process.*	In 2020 we completed a set of technologies to control batteries more smartly: printed sensors, a readout system for fast (>10Hz) reading of up to 1024 sensors and algorithms providing accurate battery state estimations based on these sensor data. A portable technology demonstrator was made. With this, the topic is now ready for further joint development with industry and is therefore terminated as ERP-topic.

16: **Appl.AI** *This ERP, our largest, consists of a coherent set of program lines, two of which being the 'flagships' of the program: SNOW (AI capabilities for self-aware autonomous systems that can operate safely and effectively in an open world) and FATE (AI to provide fair advices by continuous learning from multiple potentially confidential and biased data sources). These two flagships form the actual ERP and are surrounded by a set of use case projects.*	In 2020 we have shaped the Appl.AI program in its current form, by combining the ERP Hybrid AI, VP ICT/AI and strategic initiatives of the 2019 Appl.AI endeavor. All central activities with respect to AI are now aligned into one program. In SNOW we creating our autonomous system 'SnowBoy', build on top of the SPOT robot from Boston Dynamics In December a demonstration was given where SnowBoy was searching and assisting victims in a building. In FATE we developed a fair decision support system with Diabetes-Type 2 as leading use case. In 2020 a.o. we demonstrated the applicability of 'secure federated learning' in this use case. We have learned that use cases connected to the flagships indeed strengthen their research focus.
17: **Decarbonisation** *We target to reduce the dependency of the chemical industry (primarily at the Chemelot site) on fossil sources, by developing climate proof technologies and associated implementation strategies.*	In 2020 this program has significantly enhanced its focus on process innovation. One such focus area is the development of electrically powered plasma-chemistry, for which business models, an economical calculation model and experimental test setups were built. Another focus area concerns a plastic waste pretreatment technology that has been developed this year. By such pretreatment processes, plastic waste can be used as feedstock for pyrolysis (relevant to several Chemelot-based companies).
2nd year projects: Start 2020 – End 2023	
18: **Body-Brain Interactions** *We improve life-long health, performance and mental strength via mechanism-based understanding of the connections between body and brain, realized into a Brain-Body Interaction technology platform.*	We developed a new way of sampling small aliquots of human blood (using a preclinical technology known from research with mice) to enable human profiling and characterization. We will use this technology with the human volunteers in the human Body-Brain platform on molecular level. An approved METC experimental design was made for the study on sleep deprivation as an acute stressor.
19: **Social XR** *We create a shared XR environment, where participants get an enhanced feeling of being in the presence of, and interacting with, other persons at a remote location.*	We have built a proof-of-principle of automated calibration and synchronization of a networked multi-camera configuration, resulting in improved eye-contact. We have developed a Tactile Proxy (data streaming format) between our VR environment and Tactile displays of various types and modalities. We have built a proof-of-principle of the instantaneous, automated and orchestrated deployment of Social-XR processing modules on edge computing and cloud infrastructures, including flexible processing of the media streams We have built a test setup that allows for experimentation with different 5G mobile networking scenarios.

In addition to the Full ERP programs we executed 6 Seed (single-year) ERP projects (see Table 2 below). Our policy is to yearly execute a set of such Seed ERP's, of which a selection based on quality and outlook is promoted to Full ERP's for the four years thereafter. In the course of 2020 the Seed ERP's "Climate and Air Quality" and "Circular Structures" have been promoted to Full ERPs starting in 2021.

Table 2. Seed ERP's Highlights 2020

Seed (single-year) ERP's	
(Link to) Chapter: ERP-title *Short description*	Highlights
2020 → promoted to Full ERP, 1st year projects: Start 2021 – End 2024	
20: **Climate and Air Quality** *We develop a globally applicable, multi-scale atmospheric modelling system with resolution down to 25m to fully exploit the emerging observation capacity from satellites and sensors.*	We realized a functional and practical design of the modelling system. We have demonstrated the potential of high resolution atmospheric modelling in the DALES tool, combined with detailed NOx emission data from traffic.
21: **Circular Structures** *We develop knowledge and technology that enables for concrete structures a shift from traditional design strategies to a new engineering design method driven by supply quality-demand integration.*	We demonstrated our approach to sustainable design of concrete structures (aimed at minimising depletion of natural resources, CO2 emission and LCC) by using optimisation algorithms in the TNO EVEReST tool. We developed a method to integrate quality data in the evaluation (from circularity perspective) of resistance and durability of concrete structures.
2020	
22: **Solar2Hydrogen** *We study the manufacture of a fully integrated H_2O conversion device in which light harvesting, charge separation, and catalysis can be unified to produce H_2 in a single step, leading in turn to low(er) investment costs.*	We assessed the potential of the solar-to-hydrogen concept, in which solar energy is used to split water into oxygen and hydrogen. Various concepts with different degrees of integration of the photovoltaic and the electrolysis functionalities were compared from technical and economical perspective. We demonstrated that we are capable of making lab scale devices for photoelectrochemical water splitting, and that photoelectrochemical water splitting has the potential to provide access to green hydrogen at lower cost that electrolysis.
23: **Business Models for Transition** *We explore how collaborative business models can be used to shape and accelerate transition towards sustainability*	We have developed a research agenda for Collaborative Business Models for Transition (CBM4T), identifying relevant topics for fundamental and applied research. We have performed an analysis across 3 cases leading to identification of 5 properties for CBM4T-methodology.
24: **Human Capital** *We build up skills-based human capital strategies that enable effective up- and reskilling and intersectoral mobility of human capital.*	We have built an approach to make the existing semi-static skills ontology dynamic with regard to changes in skills and to changes in labour market needs. Based on use cases, we have developed a skills-based instrument and intervention for innovative human capital strategies.
25: **Energy Modelling** *We build up a suite of energy models and methods on different geographical levels to support decision makers in the energy system with reliable and up-to-date insights.*	We have explored the energy modelling needs, the current modelling base at TNO and the most important new modelling principles in the domain of energy. We have developed a research agenda with key research questions in the frame of the Energy Transition that TNO should be able to answer over the next 5-10 years

In the frame of the above described ERP programs opportunities to publicize and to patents results were actively pursued. Overall the ERP programs yielded a total of approximately 90 scientific publications and 170 other publications. A total of approximately 20 patents first filings was done.

In 2020, we shared our plans and results of this year and of previous years with many potential partners and stakeholders in the form of patents and other publications, conference presentations, posters and ERP dissemination events.

In the next chapters the progress in these ERPs is described in a concise form, agreed with the ministry of Economic Affairs and Climate, including a description of the setting of the research in national and international context, highlights of results obtained, cooperation in the ecosystems that we pursue, use cases and contextual dynamics. The ERP plans for 2021 and beyond are described in 'TNO Early Research Program Annual plan 2021' (reference TNO 2020 S083, dated October 5th, 2020).

2 ERP Quantum Computing

ERP Contacts: K. Eijkel (Project Lead), R. Versluis (Lead Scientist), C. Hooijer (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

Quantum mechanics is the theory to describe the (interaction between) elementary particles. Academic research has confirmed the validity of this intriguing theory as well as many of its counterintuitive aspects. But only due to recent breakthroughs is it possible to demonstrate important quantum mechanical concepts on systems large enough to be usable to humans. The concepts of 'superposition' and 'entanglement' can now be exploited, and thereby open the path to applications like the Quantum Computer with unprecedented computing powers for specific problems, and communication which is inherently safe from eavesdropping, called Secure Quantum Internet.

A Quantum Computer shall finally provide society with a tool to solve some of the Sustainable Development goals as defined by the United Nations: For example, the development of room-temperature superconductivity could provide us with lossless energy transport and storage which in its turn solves our energy shortage problem. The development of new medicines will be done by rigorous calculations instead of trial and error, which reduces both costs and time. Commercial applications may include software validation, airplane design, data search, and encryption. Encryption and secure quantum communication are also of great interest to defense organizations. Besides this societal and economical motives for application of quantum technologies, a new supply chain/industry has to be set up for manufacturing of the quantum computer and secure internet.

This vision is backed up by the Nobel Prize Committee: "Perhaps the quantum computer will change our everyday lives in this century in the same radical way as the classical computer did in the last century.", as well as by multi million euro investments by companies (Intel, Microsoft, IBM, Google) and nations (Netherlands, USA, China, UK). The European parliament and its related organizations consider quantum technologies as the only viable candidate for a large-scale European investment since the Graphene and Human Brain flagships. In this challenging environment TNO is well positioned due to the partnership with the TU Delft called QuTech, and intense cooperation with Microsoft and Intel.

Due to the technology involved as well as due to the relevant industrial players, i.e., potential customers of TNO, quantum technologies could be regarded as an extension to the TNO's Industry Semicon Roadmap. Quantum Technology has recently been added to the International Technology Roadmap Semiconductors roadmap, and also as an extension to the technology portfolio of the TNO Unit Industry. Nanofabrication for quantum computing, for example, generates new knowledge that could also be relevant to TNO's existing partners in the semiconductor industry. Challenges in encryption and secure communication make this project also of interest to TNO's ICT and Defense Units.

Results realized

No.	Results planned	Realization
1	A1 InSbAs 2DEGs multi-terminal island devices and test reports	Yes. Several island devices have been produced and characterized. The measurement results are very promising.
2	A2 new Kwant release, including Poisson solver interface	Yes. A new version of Kwant has been released.
3	B1 wafers (SiGe for silicon and germanium quantum wells) for PhD's and workflow for wafer fab.	Yes
4	B2 transmon qubit chip design.	Partly. Finalization in 2021.
5	B3 Central Controller (CC) including real-time error decoders and real-time feedback control for S17	Yes
6	B4 new OpenQL release	Partly. Has been started, final release in 2021.
7	C1 NV center for the Quantum Internet Demonstrator and workflow for NV center fab	Yes
8	C2 Review and steer the ICON collaboration	Yes
9	C3 monolithic cavity for quantum memory research and workflow for cavity fab.	Yes. Although COVID-restrictions caused significant limitations.

10	C4 fiber-pigtailed mount for quantum memory research	Yes. Although COVID-restrictions caused significant limitations.
11	C5 new Netsquid release	Yes
12	C6 Develop a process for the fabrication of NV center devices, including a number of test devices	Yes. The main process steps have been developed (although some improvements are still required), and a first complete test device has been produced.
13	C7 locking scheme to reduce the vibrations of Demonstrator set-up	Partly, delayed by Corona. Will continue.
14	D1 Web interface online using simulated quantum network, Quantum link between Delft and The Hague: 2-node system	Yes. NetSquid simulation tool launched. Quantum Network Explorer planned for Q1 2021.
15	D2 Si 2-qubit chip accessible via website or SDK to perform quantum algorithms with 24/7 access, stable.	Realized

Realized contribution to new knowledge and technology

The QuTech program has created in depth know-how and insight in quantum technology needed for quantum computing and internet. TNO's Quantum Technology, Radar Technology, Opto-mechatronics as well as Optics department have gained a track record of showcases of creating high quality quantum technology. In January 2019, an external review committee consisting of internationally esteemed scientists, chaired by Robbert Dijkgraaf, has judged the research at QuTech as 'excellent' and world leading. We are preparing for the next review, planned early 2022.

Together with other national players in quantum technology development, QuTech has created the National Agenda Quantum Technology (NAQT). The NAQT was presented in the Hague on 16 September 2019. The agenda describes how the Netherlands can further strengthen its globally-leading position in the coming years. The agenda works towards the following objectives:

- Connecting parties in the Netherlands to work together on common goals and challenges;
- Accelerating the economic impact of quantum technology for the Netherlands;
- Contributing to the government's societal tasks;
- Positioning the Netherlands as an international knowledge and innovation hub for quantum technology: Quantum Delta NL, or QΔNL for short.

The agenda divides quantum technology into three application areas: quantum computation, quantum communication and quantum sensing.

Realized contribution to the market position

The QuTech B2B and mixed funding revenue has been around 5Meuro in 2020 and will grow to approximately 10 Meuro in 2021, due to added activities in the NAQT, in the Fujitsu contract and in other contracts. Within the TNO-side of QuTech the multiplier is expected to raise to around 3, which is a healthy number in an ERP/SMO supported program. Although the revenue is still largely based on government funding in the developing quantum market, the position of QuTech in the market is strengthening:

- QuTech's position in the EU is very strong;
- QuTech's attractiveness to international corporate players remains very strong, leading to continued and extended cooperation;
- The local ecosystem is growing fast, with 2 spinouts in 2020, 5 in the pipeline, and almost 5Meuro of risk capital in 2020;
- The IP policy in QuTech is now in place, with target IP areas such as Germanium Spin qubits, diamond-vacancy based spin qubits, cru-electronics and MDI-QKD.

As a result, we expect a good B2B position in the medium term.

Publicity

Papers

A large number of quality papers was published in 2020. A few examples:

- Quantum Dots in an Two-Dimensional Electron Gas, I Kulesh, CT Ke, C Thomas, S Karwal, CM Moehle, S Metti, R Kallaher, Physical Review Applied 13 (4), 041003
- InSbAs two-dimensional electron gases as a platform for topological superconductivity, C Moehle, CT Ke, C Thomas, M Lodari, G Scappucci, S Karwal, S Metti, Bulletin of the American Physical Society 65
- Quantum transport simulations made easy | Kwant (kwant-project.org)

Patents

In 2020, the QuTech IP Board was launched. The first version of an IP policy was put in place, and the IP-awareness was raised from October onwards, leading to a healthy influx of IDF's. IN December, 6 new IDF's were received.

Patents in progress:

- Programmable dual-channel high frequency narrow-pulse-width electronic pulse generator, Raymond Frans Laurens Vermeulen
- User programmable system for high frequency time filtering and processing of quantum communication patterns, Raymond Frans Laurens Vermeulen
- Nanowire accumulation gate virtual mesa, Guoji ZHENG; Nodar Samkharadze
- Compensated microwave driven semiconductor qubits, Xiao XUE; Nodar Samkharadze

3 ERP Energy Storage and Conversion

ERP Contacts: N. Meulendijks (Project Lead), P. Buskens (Lead Scientist), C. Hooijer (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

The ERP Energy Storage and Conversion consists of two research lines: Electrons-to-chemicals and Photons-to-chemicals, which are subsequently presented.

Research line: Electrons-to-chemicals

The focus is on the process development for the conversion of CO_2 to C1 chemicals and fuels, mainly formic acid (FA) and CO, using renewable electricity as energy source. These small molecules can be used either as a fuel or as base chemicals. The electrochemical conversion of CO_2 to FA and CO are, based on the electron consumption, the most efficient to pursue. To be able to develop a cost effective process concept, these four main requirements need to be fulfilled:

1. Current density should be above 1 kA/m^2;
2. Faradaic efficiency should be above 50%;
3. Power consumption lower than 500 kWh/kmol;
4. Electrode lifetime should be above 8000 hrs.

The main goal of the research line Electrons-to-chemicals is to convert CO_2 to FA and CO using renewable electricity as energy source. To be economically feasible, the CO_2 capture, conversion, and downstream product processing need to be integrated into one reactor and process concept. When CO_2 has to be captured first from a dilute stream (e.g. flue gas, air capture) and purified, the cost of the CO_2 will be, depending on the source and scale, around 100 to 600 euro per ton. It is clear that, based on the current prices of FA and CO, it would be difficult to realize an economically attractive process. Furthermore, the process needs to fulfill the requirements mentioned above.

In 2018, we successfully developed two different routes for CO_2 capture. The first route is an indirect route, which proceeds via the capture of CO_2 in the electrolyte followed by subsequent reduction of the captured CO_2. The second route is a direct route, using a gas diffusion electrode (GDE) to transfer CO_2 to the vicinity of the electrode followed by subsequent reduction of CO_2 at the electrode. The second route showed the most promising results in a first comparative technoeconomic feasibility study.

In 2019, we aimed to realize a proof of concept (TRL 4) for integrated CO_2 capture and conversion using an inhouse developed continuous flow reactor with an optimized three compartment GDE based cell (see *Figure 2*).

Figure 2: Low pressure continuous flow reactor & TNO's electrochemical cell design

The demonstrated concept is based on the use of a cathode comprising a GDE in a three compartment electrochemical cell. The GDE is used as a membrane contactor to remove CO_2 from flue gas, and subsequently convert it to a non-volatile chemical. This chemical is a formate salt. Due to the fact that this has zero vapour pressure, no contamination of the treated flue gas can occur. Next to the GDE, the electrochemical cell consists of a middle compartment separated from the anolyte and catholyte chamber by ion selective membranes (i.e. anion and cation exchange membranes). The produced formate is combined with the protons produced at the

anode in this middle compartment to FA. This FA is enriched up to a concentration of ~10 wt%. Although FA can be a product of interest, the approach within the ERP considers FA as an ideal intermediate chemical for the production of high volume chemicals such as CO and formaldehyde because of the relative small market volume of FA.

Advanced modelling and dedicated experiments with in-house developed Tin based GDE already has shown potential for this approach in 2018.

In 2019, we demonstrated an integrated CO_2 capture/conversion methodology, the efficiency of this concept for very dilute CO_2 sources (i.e. air capture) was explored and a detailed techno-economic evaluation of the developed process concept was performed. For the first time in the world, TNO has demonstrated that a reactive capture medium for CO_2 can be used as an electrolyte for the reduction of the absorbed CO_2 with reasonable efficiencies. This was done based on synthetic flue gas conditions. With the obtained knowhow, we are going to demonstrate that our (patented) approach can as well be used for integrated CO_2 capture from **air** and direct conversion to value added products.

Research line: Photons-to-chemicals

The focus is on the conversion of CO_2 to C1 chemicals and fuels, using sunlight as energy source for driving the reaction. The long-term goal is to develop and validate concepts for production of ≥C1 chemicals and fuels through sunlight-fueled hydrogenation of CO_2.

In 2016/2017, we managed to successfully demonstrate the concept of plasmon catalysis in a model reaction, i.e. the Suzuki coupling of bromobenzene and p-tolylboronic acid catalyzed by Pd-decorated gold nanoantennas.

In 2018, we managed to successfully demonstrate the concept of plasmon catalysis for photochemical hydrogenation of CO_2 to methane. We designed and developed a Ru nanocatalyst, and demonstrated that it selectively converts CO_2 and H_2 to methane (CH_4) using the entire solar spectrum spanning from the ultraviolet to the near infrared. Using sunlight as energy source, we were able to perform this reaction, which normally requires a temperature between 300 and 500°C, at room temperature. For demonstration purposes, and comparative testing of various catalysts, a lab scale reaction cell was developed. This is not a suited reactor concept for scale up.

In 2019, based on the input from the companies in the business team of the Interreg project EnOp and experts from the Chemelot Campus, we focused on producing CO rather than CH_4. This conversion is expected to be economically more favourable. For that purpose, new metal nanocatalysts were developed, characterized and validated. Furthermore, we designed and established a reactor tailored for CO_2 conversion with plasmonic catalysts and sunlight as energy source.

In 2020 we have further optimized and validated the lab scale test cell for screening the plasmon catalytic conversion of CO_2 to CH_4 using artificial sunlight. We have synthesized a series of catalysts for CH_4 production, and optimized the catalyst materials with respect to activity (space-time-yield). The catalysts were fully structurally and optically characterized and validated. The reaction mechanism was investigated in more detail by studying the activity as function of the distance between the metal nanoparticles on the support, reinforced by a modelling study, indicating the collective photothermal effects play a key role in this process. These results were published [https://doi.org/10.1002/cctc.202000795]. Based on the input from the companies and experts from the Chemelot Campus, we currently are focusing on producing CO in addition to CH_4. This conversion is expected to be economically more favorable. The technoeconomics of both processes are currently being investigated. New metal nanocatalysts for the conversion to CO are developed, characterized and validated. Several types of plasmonic metals are investigated and the combination with different types of support material was tested, yielding Au supported on semiconductive TiO_2 as most promising candidate for further optimization. Furthermore, the design for a mini factory tailored for CO_2 conversion to CO and CH_4 with plasmonic catalysts and sunlight as energy source has been completed. The equipment has been ordered and the setup will be established and validated in 2021. Furthermore, in 2020 we have developed strategies for commercially feasible photo(electro)chemical conversion of CO_2 to methanol.

In 2021, the research will focus on the development and validation of the lab scale minifactory for CH_4 and CO production, and accompanying techno-economic feasibility study. In addition, focus will be on the development of efficient plasmonic catalysts for photochemical and/or photoelectrochemical CH_3OH production and ≥C2 chemicals and fuels.

The activities on CO_2 hydrogenation will be supported by selected scientific studies performed at Hasselt University (synthesis and characterization of nanocatalysts) and Zuyd University of Applied Sciences (development of flow reactors for plasmon catalysis). Furthermore, experts from the Business Team of the Interreg project LUMEN and the Chemelot Campus will be consulted with respect to technoeconomic feasibility of these processes.

The photons-to-chemicals research program fits to the 'NWA route: Energietransitie', and relates to the 'topsectoren: Chemie, Energie and HTSM'.

Results realized

Research line: Electrons-to-chemicals

No.	Results planned	Realization
1	ELEKTRA setup	Completed
2	Technical report of experimental results	Completed
3	Manuscript ELEON paper (submitted)	Completed
4	Manuscript GDE parametric study paper (in preparation)	Completed
5	Manuscript Effect of partial pressure on product selectivity in Cu catalyzed electrodes – NWO Elerecet project- published	Completed https://pubs.rsc.org/en/content/articlelanding/2020/se/d0se00865f

Research line: Photons-to-chemicals

No.	Results planned	Realization
6	LUMEN Validation of optimized plasmonic catalyst for Sabatier reaction	Completed
7	LUMEN Design of a tailored flow reactor for plasmon catalytic conversions	Completed
8	LUMEN Reverse water-gas shift reaction (rWGS).Catalyst Optimization and Validation	Completed
9	Report on the modelling study to compare shape selectivity vs activity	Completed
10	Report on commercially feasibility of photo(electro)chemical conversion of CO_2 to methanol	Completed
11	Manuscript Collective Photothermal Effect of Al_2O_3-Supported Spheroidal Plasmonic Ru Nanoparticle Catalysts in the Sunlight-Powered Sabatier Reaction - published	Completed https://chemistry-europe.onlinelibrary.wiley.com/doi/full/10.1002/cctc.202000795

Realized contribution to new knowledge and technology

Research line: Electrons-to-chemicals

In ERP 2020 some of the most promising synthesis routes from previous years were explored and advanced. More notably:

- the ELEON technology was explored further and the product portfolio was expanded to also include carbon monoxide and oxalic acid in addition to the formic acid already explored.
- Another route started in previous years in ERP was the development of gas diffusion electrodes. The classical route of making gas diffusion electrodes has been perfected further to the content of catalyst loading and ionomer. In the process intensification work package a novel gas diffusion electrode configuration was put forward as a more robust alternative to the current commercial solutions which are adapted from water electrolysis. This novel concept is currently part of a patent application.
- The three-compartment electrolysis idea was also advanced in ERP2020 and made more efficient by replacing the ionic conductive media in the middle compartment with a polyelectrolyte. This novel idea was included in a patent application in 2020.
- One completely new concept which was not explored in previous years in ERP was brought forward this year and this is the electrolysis of CO_2 in an undivided cell. The one compartment electrolysis was showed to lead to a feasible formic acid production which can be integrated with a continuous formic acid extraction. This new process idea also led to a patent application.

Interreg Power to Fuels 2020 - with this project, TNO will gain:

- A world class unique test infrastructure on integrated CO_2 capture-electrochemical conversion
- Knowledge on electrochemical engineering
- Knowledge on system development
- Knowledge on integrated product separation
- Knowledge on electrocatalyst characterization and performance determination
- Knowledge on electrochemical reactor design
- Knowledge on business cases related to electrochemical CO_2 conversion

The visibility of TNO within academia and industry have been substantially improved (via congress presentations, via the VoltaChem program and via the initiation of new joint research projects). In conclusion, it can be stated that our position on electrochemistry has been substantially improved. By aligning the ERP work with the VP Chemistry on electrochemistry, a broad coherent electrochemistry program has been created at TNO.

Moreover, the industry day organized for presenting the plans for a shared research program around the integrated CO_2 capture and electrochemical conversion has attracted the interest of over 25 companies relevant both in the technological as well as in the value chain of this technology.

Research line: Photons-to-chemicals

Photochemical conversion of CO_2 to C1 chemicals/fuels using sunlight as energy source:

ERP2020: Strategies of commercially feasible photo(electro)chemical conversion of CO_2 to methanol

Interreg LUMEN:

- Further development and validation of the batch reactor for plasmon catalytic conversion of CO_2 to CH_4.
- Optimized catalyst for plasmonic photoconversion of CO_2 to CH_4 with respect to activity/space-time-yield (STY).
- Development of a library of catalysts for the conversion of CO_2 to CO.
- Variation of plasmonic metals.
- Optimized NPs size and shape to increase the light-harvesting and the production ration
- First design of complete lab scale mini-factory for the conversion of CO_2 to methane and CO.

With this project, TNO will gain:

- A unique technology for further exploration in the field of chemical energy storage.
- A portfolio of nanoparticle catalysts/new knowledge in the field of synthesis and characterization of metal, dielectric metal oxide and semiconductor nanoparticles.
- A unique technology for using solar energy in applications in which sunlight needs to be collected and converted into fuels or intermediate chemicals.
- Knowledge on the interaction of (metal) nanostructures/particles with light.
- Knowledge on business cases for solar fuels and photochemical water splitting.
- Knowledge on photonic devices for solar fuels and design of tailored reactors for plasmon photocatalysis

Strong position of TNO on photochemical conversion of CO_2 to C1 chemicals/fuels using sunlight as energy source. The visibility of TNO within academia and industry has been substantially improved (via congress presentations, via the Nanotechnology crossing borders event, via the Interreg program LUMEN and via the initiation of new joint research projects like the granted H2020 project SPOTLIGHT). This has led to new initiatives like the H2020 RADIANT project proposal which was submitted in August 2020 and the development of TKI projects MAT4CAT and FLuxChem.

The relevance of the results for the governmental departments or companies/organizations involved concern:

- catalyst producers: new types of catalysts to add to their portfolio
- chemical companies: new processes for green hydrogen production and CO_2 conversion to C1 chemicals/fuels using sunlight as energy source
- specialty chemical companies: new photocatalysis concept for production of fine chemicals
- equipment manufacturers: new tailored reactors for photochemical reactions using sunlight as energy source.

Realized contribution to the market position

Research line: Electrons-to-chemicals

By establishing an extensive electrochemistry test and analyses infrastructure, TNO has a unique position, certainly in the BENELUX, but to a lesser extent in Europe, on process development using electrosynthesis. International companies such as Perstorp and AVA recognize our knowledge position. First market penetration has already occurred. It is to be expected that our efforts will lead to a substantial increase of spinoff projects, both B2B as well as EU/TKI/INTERREG co-funded projects.

The new installations (ZEUS, ELEKTRA) which are in the course of being built will be part of a FIELD LAB setup up in the region of Zuid Holland. Around the field lab, a center of excellence will be created which will allow an

active collaboration between companies, TNO and other interested parties in the technological developments related to the valorization of CO_2 using electrochemistry.

For the commercialization of the results of the project, under the VoltaChem program umbrella, targeted dissemination is being done. This has created more awareness in the outside world on the capabilities of TNO and has attracted parties wanting to commercialize the technology. All business development is done via the Sustainable Chemical Industry Theme line with full support of two business developers. To keep the market focus of the research, the VoltaChem program management is also done via the Theme.

Recent examples of commercialization activities are: A H2020 VOLTAFERM project proposal including the one compartment electrolysis idea, an H2020 project proposal was formulated for the demonstration of the ELEON technology, an ERA NET project proposal was submitted for the development of the ELEON technology. Furthermore a B2B project for Total, with the aim to build a setup for reduction of CO_2 was proposed. Several NWO sponsored fundamental research projects on CO_2 reduction to various products is supported by TNO; a community of companies has been built around the VoltaChem brand and program to be able to directly get feedback and generate new opportunities for electrification (http://www.voltachem.com/community). The knowledge needed for all these activities has to a large extend been generated in the ERP E2C program. Additionally an advisory board has been established populated by representatives of academia and industry to get feedback and steering on the research done in the ERP E2C at the same time also giving opportunities for further joint innovation and commercialization.

In 2019, the first communities of practice meeting was setup up. Companies which are part of the Voltachem community have gathered at TNO where our electrolysis technologies were presented by the team of scientists. This meeting was the prelude for the follow up Industry day at the end of November where the focus was put only on one of our technologies: Integration of CO_2 capture and electrochemical conversion.

In 2019, the organization of the Industry day was the notable event which gathered more than 25 relevant companies interested in electrolysis of CO_2, CO_2 valorization, CO_2 capture and utilization. The technology put forward for the development of a shared research program is the Integrated CO2 capture and electrochemical conversion.

In 2020, an investment project was granted to TNO to advance the infrastructure on integrated CO2 capture and electrochemical conversion. These installations are being purchased part of the Field lab industrial electrification.

Research line: Photons-to-chemicals

This ERP contributes to the improvement of the market position of TNO (turnover, customers) by:

- Unique technology in the field of chemical energy storage
- Multiple academic and industrial partners involved via Interreg program LUMEN
- Unique technology in the field of solar fuels.

Concerning the commercialization of the results of the project the following actions have been taken:

- Ongoing discussions with companies in the user committee of the Interreg project LUMEN and experts from the Chemelot Campus
- Industrial partners involved via Interreg program LUMEN and H2020 project SPOTLIGHT

After analyzing the results, publishing in scientific journals have found more interesting and useful. The existing patent (No. 201480035493) has been expanded with a divisional for CH/JPN.

Publicity

Research line: Electrons-to-chemicals

Scientific Publications:

- Effect of partial pressure on product selectivity in Cu-catalyzed electrochemical reduction of CO2, Sustainable Energy Fuels, 2020, 4, 5195
- The AIChE Netherlands / Belgium Section, Dinner lecture, Technology integration: CO2 capture and conversion: A comparison between an electrochemical and a thermocatalytic route

Patents/IP:

- Electrochemical production of hydrogen peroxide, International Patent Application No. PCT/NL2017/050421
- Electrooxidation of propylene glycol to lactic acid – International Patent Application P115848EP00 - 2017010 II/SCI # 52041011
- Electrochemical reduction of levulinic acid – provisional patent application (in progress)
- Integration of CO2 reduction with selexol solvent absorption / capture (in progress)
- Three compartment strategy for the conversion of CO2 to formic acid and oxalic acid (in progress)
- Electrolysis of CO to formaldehyde and ethylene (in progress)
- Integrated heat utilization and CO2 stripping (in progress)
- GDE engineering using dense membranes (in progress)
- CO2 electrolysis in undivided cell and DSP (in progress)
- Electrochemical production using a polyelectrolyte P126947ER00

Research line: Photons-to-chemicals

Scientific Publications:

- Roos Grote, Roberto Habets, Jelle Rohlfs, Francesc Sastre, Nicole Meulendijks, Man Xu, Marcel A. Verheijen, Ken Elen, An Hardy, Marlies K. van Bael, Tim den Hartog, Pascal Buskens, Collective Photothermal Effect of Al2O3-Supported Spheroidal Plasmonic Ru Nanoparticle Catalysts in the Sunlight-Powered Sabatier Reaction. ChemCatChem 2020, 12, 5618 (incl. cover picture).
- Bob van der Zwaan, Remko Detz, Nicole Meulendijks, Pascal Buskens, Renewable Natural Gas as Climate-Neutral Energy Carrier?, Environmental Science and Technology, submitted for publication.

Presentations at conferences and symposia:

- Oral Presentation “Low temperature solar CO2 methanation” Francesc Sastre, Roos Grote, Nicole Meulendijks, Ken Elen, Marlies k. Van Bael, Tim Hartog, Marcel Verheijen, Pascal Buskens in the 14th Mediterranean Congress of Chemical Engineering (MeCCE-14) held virtually from November 16th to 20th, 2020.

Patent descriptions, premier depots.

- U.S. Patent Application No. 14/892100 – ‘’Plasmon assisted bulk chemical conversions”

4 ERP 3D Nano-manufacturing Instruments

ERP Contacts: J. van Driel (Project Lead), S. Bäumer (Lead Scientist), C. Hooijer (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

There are already more connected devices than there are people on the planet and the demand for these devices is steadily increasing: IOT, connected cars, immersed reality (virtual and real world augmented). All of these products and applications rely heavily on semiconductor devices. With increasing needs for production of ever smaller and faster devices, the semiconductor industry is currently facing major challenges on manufacturing, metrology and testing. To accommodate the demands, the semiconductor manufacturing is quickly shifting away from planar device configurations and is moving towards 3D or stacked structures, such as multi-gate logics (e.g. FinFETs, Gate-All-Around FETs, and nanowires) and 3D NAND memories with still shrinking pitches, see also *Figure 3*.

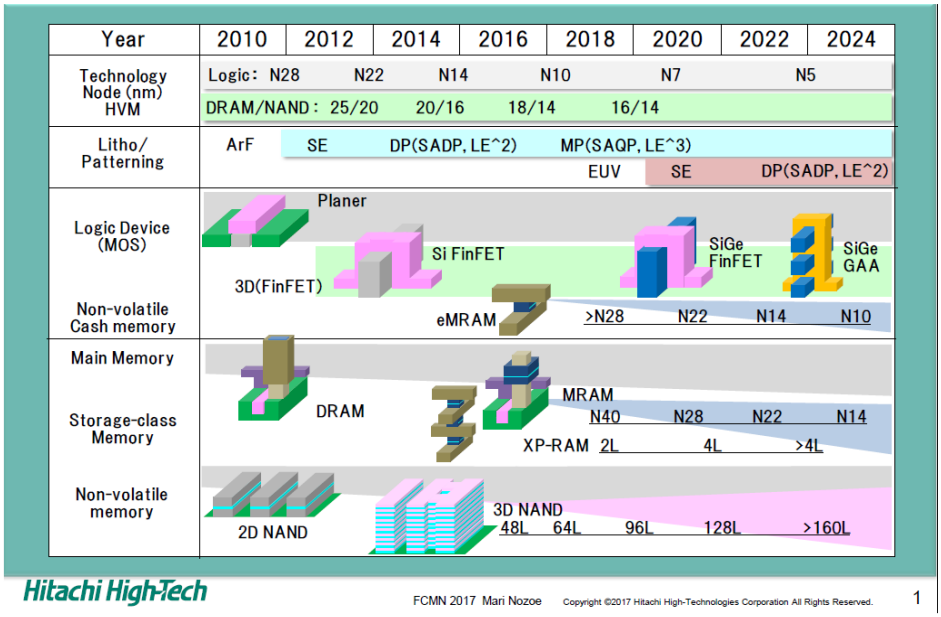

Figure 3: *Developments in semiconductor manufacturing.(Mari Nozoe, Hitachi)*

Due to the increased geometrical, processes and materials complexity and the continued shrinkage, the conventional metrology and device testing techniques are running into their limits in terms of both sensitivity and resolution. Therefore, development of non-destructive techniques that are able to image, measure and characterize nanoscale production features even through multiple and optically opaque layers are essential for production of the next generation of semiconductor devices.

TNO has gained substantial experience in Scanning Probe Microscopy (SPM) as one of the promising solutions for measuring defects and dimensions of 2D and 3D structures. Because the devices are moving from 2D to 3D structures, it is essential that the SPM capabilities are being extended to 3D imaging and tomography. Developing the 3D capabilities will therefore play a central role in this ERP and will be pursued through two complementary routes: 1. Mhz and Ghz subsurface imaging of the samples and 2. Photo-thermal Acoustic Imaging (PTAI). The overarching goal is to develop these techniques to give reliable and quantitative 3D information. Besides implementing 3D imaging, improvements are needed in repeatability & reproducibility of the results and for protecting the samples from damage. The latter two can be achieved through specialized control mechanisms which will be developed and demonstrated during 2019 - 2021.

The semiconductor industry is moving towards new parameters which need measurements as well. With a small exploration budget new parameters and techniques have been scouted in 2019 and assessed on their feasibility. Since the feasibility of these topics was given – at different stages of TRL - in 2020 these new modalities have been added to the initial research line of SPM. Note that the challenge of measuring extremely small dimensions with sufficient resolution and accuracy is, of course, not exclusive to semicon industry. Highly sensitive

nanometer resolution imaging will likely find applications on biomedical and biochemistry technologies (soft and sticky material characterization).

The main objectives of this ERP (2018-2021) are listed below. The color bar indicates overall progress.

- True 3D metrology / tomography of advanced semiconductor devices aiming at 1nm resolution for new nanowire and gate all around devices as well as stacked memory.

- SPM-based subsurface metrology quantitative and able to detect up to > 20 µm deep structures with a resolution of < 3 nm and able to detect horizontal gate-all-around wires.

- Advanced control algorithms, making SPM technology more repeatable, better performing, operator independent and thereby HVM fab compliant.

- Explore new trends in metrology, and where feasible go beyond, such as chemical imaging, quantum sensing and Artificial Intelligence (AI) for interpreting data.

- Expand into other application fields such as bio-detection and photonic integrated circuits being a center of excellence together with partners in academia and industry.

The defined long-term goals directly supports the future industry needs:

- 3D NAND: increasing number of stacks need overlay metrology by (acoustics) nano-tomography;
- Future LOGIC 3D integration: on product metrology for alignment and CD metrology by nano-tomography;
- LOGIC (and memory) needs for chemical properties characterization;
- Multimodal imaging: several modalities are needed to characterize the devices. In addition AI for data processing and a new ways in system engineering in combination with AI: Design for AI.
- Quantum sensing: preparing for future generations of computing and new modalities such as conductivity measurements and magnetic devices

To meet these long-term objectives, the work in 2020 focused on the following topics:

- Nanometrology and nano-tomography:
  - Subsurface nanoimaging on resolving the depth and structure of features. In particular, on Photothermal acoustic imaging (PTAI) for on-product metrology and Scattering sub-surface scanning probe microscopy (S-SSPM)
  - A feasibility study into chemical imaging.
  - Build the first TNO quantum sensing AFM

- First steps in the direction of understanding the use of AI not only in data processing but also in AI were taken: Design for AI

Results realized

Sub Surface Probe Microscopy

No.	Results planned	Realization
1	Top actuated SSPM - Deliverable 1: Proof of experimental feasibility on deeply buried markers (3 µm wide Si markers buried below 2.6 µm SiO2, or 0.8 µm pitch Si markers buried below 5 µm PMMA)	Partly achieved. 1/ Measured piezo sensitivity (by TNO) of piezo devices on test wafer within factor 3 of calculated sensitivity at the fundamental resonance frequency (~6 GHz) Acoustic stack design optimized, initial process flow defined, test chips manufactured, pulse-echo and electrical measurements performed, signal measured, cantilevers currently being manufactured, first sample measurements are scheduled for December 2020.

		Remaining test in 2021: When the subsurface markers in the samples are successfully measured using the novel cantilevers, the fundamental experimental feasibility of the method has been established.
2	Top actuated SSPM - Deliverable 2: Report on optimal approach to improving scan speed by 25% including associated scan speed estimate	Achieved through SNR optimization. Report is Powerpoint ppt format. (report and/ or paper will follow once measurements are completed)
3	Top actuated SSPM - Deliverable 3: Report on optimized design of cantilever, electronics, pulsing schemes, and signal processing	Achieved, Report is in powerpoint ppt format. (report and/ or paper will follow once measurements are completed)
4	PTAI: Report on imaging/measurement algorithms for complex samples (i.e. samples where top layers have a thickness in the order of a wavelength)	Achieved, report in Doc format with references to presentations etc.

Chemical Imaging

No.	Results planned	Realization
1	Investigate the two main contributions to chemical imaging contrast	Achieved: Both contributions (hypotheses) have been explored in simulations. Their dependence on time and tip-sample distance have been quantified.
2	Experimental verification of findings from deliverable 1.	Mostly achieved: Final verification based on experiments is pending due to limited time since system arrival and due to corona restrictions. First indications are that contrast mechanism is mainly thermal expansion.

Quantum Sensing

No.	Results planned	Realization
1	A functioning shear force AFM where the tip can approach the sample and a control loop for the tip sample distance;	Achieved. We have developed the shear force AFM, implemented the control loop and successfully approached the probe on to a reference sample and performed a topography scan over the sample.
2	Optical transmission losses determined from the laser to the tip and from the tip to the detector	We have completed the optical design to excite the probe with the laser, collect he fluorescence from the tip and image the probe and the sample on to the camera. We have determined the optical loss pathways and updated the optical setup to increase the transmission efficiency.
3	A mechanical design that can house the AFM, optical components, and microwave	Achieved. We have a mechanical design housing the AFM, optical components and microwave that follow the requirements.
4	A design for the microwave and the power delivered to the tip	Achieved. We have two designs for microwave antennas capable of providing the requested power and stability.
5	Performance test of the probe's fluorescence as a function of the microwave frequency. This is given by the number of photons emitted per GHz, which is a measure for the efficiency with which we are addressing the NV center and reading it out.	Achieved.

Artificial Intelligence

No.	Results planned	Realization
1	Use-case selection and generation of training data and test data for later AI use.	Achieved. The use case consists of a diffractive optical element optimized to allow a neural network to extract parameterized wavefront information from a single image. The virtual setup is completed. Training data and test data can be generated. It is now possible to obtain complex diffraction pattern not recognizable by simple pattern recognition.
2	Development and training of a neural network making use of established ‘building blocks’ from Intelligent Imaging The process is designed for AI.	Achieved. The first proof of principle for training consists of three convolutional layers for 5 Zernike's coefficient (target is 10 Zernikes). Results show that the training and optimization of the diffractive optical element (SLM) in some cases is necessary to recover the input Zernikes

3	Resolution of arbitrary inputs from selected use-case within required classification accuracy (> 95%), which is a metric for the evaluation of the quality of the neural network implementation and the efficiency/completeness of the training for the deep learning.	Partly achieved. The phase plate is an optimizable layer in the network, and trainability can be enabled/disabled. The classification matrix is currently based on the RMSE loss. very good performances for low complexity input (RMSEloss ~ 0.005) and performances deteriorate with increased complexity (successful mid complexity ~0.025, unsuccessful high complexity ~0.25) . Random initialization is intrinsically optimized for the neural network, and therefore there is not much use in training the SLM or not. The use case is dismissed. A global characterization of the AI with classification accuracy (number of correct predictions versus total number of predictions) has not been provided.
4	Conceptual understanding of the dependencies/effects in the implementation of a process designed to make use of AI, identifying the "most information-carrying intermediate output" as the basis for the best performing AI-based processing.	Achieved: evaluation of some effects of the neural network dependencies (example: new choice of the propagation distance) and understanding of the solutions given by the neural network, both the "known concept" and the "optimized concept". But current use case has a limited sub-optimal solution and it was decided not to start the design-for-information process (identify an intermediate output in the network layers for a faster/understandable optimization strategy) . An alternative use case (FlexIQam) is proposed for 2021. All lessons learned are condensed in a report.

Realized contribution to new knowledge and technology

To support the development of 3D nano-electronics, this ERP is developing key technologies for the metrology of nanostructures, hence process and quality control. Highlights for 2020:

In particular for SSPM, the following new expertise and experience have been acquainted:

- Knowledge on the modeling of 5+ GHz piezo transducers obtained
- Knowledge on the fabrication process techniques required to develop and manufacture piezo integrated cantilevers at 5+ GHz obtained
- Knowledge obtained on how to design 5+ GHz piezo transducers within the limitations of the suitable fabrication techniques
- user friendly and versatile simulation tool for acoustic wave interaction with materials at nm scale
- Knowledge obtained regarding possibilities and (possible) limitations of using forward modelling capability for quantitative imaging
- Feasibility of 5+ GHz piezo transducers built using production process compatible with AFM cantilever production process established
- Experimental feasibility established of electrically interfacing 5+ GHz piezo transducers in a practical manner.
- Limitations of cantilever PTAI system are explored and documented

IR-AFM measurement method for chemical imaging:

- Simulation framework covering relevant physics for IR-AFM. This allows both to improve and finetune the method, but also to predict and guaranteed performance of this technology for particular applications.
- We have started building up experience on applying IR-AFM to different types of metrology and research questions relevant for upcoming semiconductor nodes (e.g. DSA, ALD, EUV mirrors and pellicles)

During 2020, we got acquainted with a large range of technologies while developing the QSPM prototype, those including MW control and measurement, and NV technologies.

The following expertise and experience have been acquired in the research line AI:

- Knowledge on the modeling of a complex (not real) neural network
- Knowledge of coding in PyTorch to use matrix multiplication to speed up simulation code

Because of this ERP, the technology position of TNO has improved further. The progress made in several disciplines have already proven to be used and useful in in number of projects and disciplines:

- Acoustic modelling and data retrieval is being used in several research and customer projects.
- Photo Acoustic Sensor which is develop in cooperation with CAS (CEE)
- Opto-acoustic sensors: PIC based / Distributed Acoustic Sensing

Regarding the possible applications of the QSPM, we internally submitted or are preparing to submit the following invention ideas:

- Semiconductor metrology using diamond NV center based sensors (PLT 2020098)
- Semiconductor dopand profiling using diamond NV center based sensors
- Defect inspection for semiconductor industry using NV center based sensors

Realized contribution to the market position

The ERP SSPM program on integration of piezos on customized cantilevers created further interest with a large equipment manufacturer. A project was kicked-of that builds on the knowledge built in the ERP.

PTAI: B2B project in acoustic microscopy (semicon application)

Turnover generated in 2020 with B2B projects based on high frequent acoustic metrology and AFM surface metrology are well beyond 1MEUR.

The concepts being developing for Chemical Imaging is already gaining traction from a large ODM. This company has shown interest for TNO to perform custom sample measurements to investigate the capabilities for the fairly novel method for process and quality control. Furthermore TNO participated with this technology in the IT2 project with a turnover of on average 330kEUR / year for the next 3 years.

The AI program is not yet in the position to directly contribute to the market position of TNO, but shows that is a potential game changer for the majority of our work at TNO. Changes to the system engineering approach, different resources and a different way of work would be required and this would take time and practice, but once industry finds that the gain in performance outweighs the loss of explainability it may go faster than conventional design.

Finally, the know-how and expertise developed within this ERP enabled participation in the ECSEL proposals IT2 and Hifidelity. IT2 was granted at the end of 2019, and HiFidelity was submitted in 2020 but unfortunately not granted.

Publicity

Scientific publications

- D. Piras, P.L.M.J. van Neer, R.M.T. Thijssen, H. Sadeghian, ‘On the resolution of subsurface atomic force microscopy and its implications for subsurface feature sizing’, Rev. Sci. Instrum., 91(8): 083702-1-10, 2020, https://doi.org/10.1063/1.5140427.
- M. H. van Es, B. A. Quesson, A. Mohtashami, D. Piras, K. Hatakeyama, L. Fillinger, P. L. van Neer, Bottom Actuated GHz Subsurface Scanning Probe Microscopy: experimental validation, arXiv:2007.01662 (2020).
- M.H. van Es, B.A.J. Quesson, A. Mohtashami, D. Piras, K. Hatakeyama, L. Fillinger, P.L.M.J. van Neer, ‘High resolution acoustic metrology by combining high GHZ frequency ultrasound and scanning probe microscopy’, Proc. SPIE 11325, Metrology, Inspection, and Process Control for Microlithography XXXIV, 113250C (20 March 2020); https://doi.org/10.1117/12.2552030.
- M.H. van Es, B.A.J. Quesson, A. Mohtashami, D. Piras, K. Hatakeyama, L. Fillinger, P.L.M.J. van Neer. “Scattering contrast in GHz frequency ultrasound subsurface atomic force microscopy for detection of deeply buried features”. rXiv:2007.01662; https://arxiv.org/abs/2007.01662; (this is the paper blocked by NFI, submitted to nature communications and rejected, then published online on arxiv, but is not peer reviewed)
- Rodolf Herfst, Maarten van Es, Stefan Kuiper, Gert Witvoet, Joost Peters, Rob Willekers, “Large dynamic range atomic force microscope”, Mikroniek 2020 – 6, 12 – 17, (2020)

Patents:

PLT2020098 Semiconductor metrology using diamond NV sensors

IP co-applied with an external industrial partner:

- IDF 2020D00573 IDF_GHz_SAM_Algorithms_fkFiltering

- IDF 2020D00723 IDF_GHz_SAM_Algorithms_Grating_Lobe_Phase
- IDF 2020D00724 IDF_GHz_SAM_Algorithms_Grating_Lobes
- IDF 2020D00725 IDF_GHz_SAM_Algorithms_Migration
- IDF 2020D00726 IDF_GHz_SAM_HardwareIDF 2020D00xxx IDF_TNO_GHz_Mark_Design

The TNO Semicon Innovation Day, which was planned in May 2020 was cancelled due to COVID – 19. This would have been the usual place to demonstrate the results to the external public as it was done in 2019 and the years before. For 2021 the SID will be held again (face to face or online). Next to the TNO SID several other conferences we planned to attend were cancelled as well.

5 ERP Personalized Health

ERP Contacts: Marjan van Erk (Project Lead), Suzan Wopereis/André Boorsma (Lead Scientist), Paulien Bongers, Paul Havinga (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

Currently, our society nudges citizens to live an unhealthy life resulting in chronic (preventable) lifestyle-related diseases and our healthcare system is equipped to manage health problems and diseases. Especially for lifestyle related diseases, evidence is mounting that lifestyle changes have a profound effect on disease progression and even disease remission or reversal is possible. Changing lifestyle behaviour is difficult; personalization, i.e. tailoring to an individual's needs and preferences, is be an important factor for achieving sustainable healthy lifestyle habits.

ERP Personalized Health develops biology and research methodology innovations for personalized health optimization. The innovations in this ERP are pivotal in the envisioned disruptive change that will result in a higher quality of life and lower healthcare costs.

Line 1: Biology

The goal to develop both the technology to measure inflammatory resilience and the knowledge of intervention strategies to optimize low-grade inflammatory resilience, thereby preventing, reversing and curing life-style related diseases with an inflammatory component. The combination of metabolic knowledge with innovative knowledge and application of inflammation within this ERP will take the personalized systemic approach of health optimization to a next level. We expect the technology from this ERP Personalized Health to be mature enough at the end of 2021 to be developed further in PPS projects in 2022 and onwards.

In 2020 the aim was to integrate the different technologies and work towards a human Proof of Concept study (hPOC) in 2021, in which technology from both WP1 and WP2 will be combined. These are the intended results and deliverables for WP1 2020:

- Description of differential and shared pathways in liver and fat tissues responding to lifestyle interventions in mouse
- Validated innovative biomarker panel from tasks 1.5 and 1.2 in samples from both human and mouse studies
- Identification of compounds for modulating inflammation by applying the Mycobiome screening technique and the Systems
- Biology Intelligence (SBI) platform
- Identification of novel nutritional analogues by applying TargetTri tools using the compounds from the Mycobiome and SBI
- platform as input for new intervention strategies.
- Protocol for analysis of microbiome/mycobiome in the hPOC study
- Draft protocol for the hPoC study by integrating WP1 and WP2 knowledge and technology (to be conducted in 2021).

Line 2: Research Methodology innovations

To achieve personalized health optimization, research methodology innovation is essential. In this research line we focus on development of state-of-the-art technology and connect these innovations to the Personal Health Advice System (PHAS), which is focused on lifestyle related health. By 2022 we aim to have developed a set of concepts and building blocks for a world-leading personal health advice system (PHAS) for all aspects of lifestyle related health and diseases. New as compared to the previous developed advice systems that were mainly knowledge-based, is 1) the innovative way to combine biological, behavioral and socio-psychological diagnostics and interventions in one system and 2) the application of new modeling techniques. The new models can be applied on the individual level, as well as within communities. The system uses "content" (knowledge, rules, models) in an architecture to collect and manage user data. The PHAS system services as a generic backbone for multiple digital techniques that provides diagnosis, advice and support and monitors behavioral change to improve and maintain a healthy lifestyle, both directly to patients/citizens and to healthcare professionals.

A key factor for success of personalized health optimization for patients and citizens is to be in control over personal health data. Within this ERP, we build the fundaments in order to initiate, facilitate, and to test “personal health data valorization” in a prototype research and health community that empowers citizens to achieve a sustainable lifestyle change. Key here is citizens empowerment through ‘personal health data valorization’ via community driven health data marketplaces, which will be in place by 2022. Simultaneously, we will include the system around the citizen/patient by setting-up the building blocks for systems-based behavioral change tooling. Our initial use case is type 2 diabetes (T2D) patients and their communities. By 2022, this will have resulted in a systems toolbox for sustainable behavioral change exploiting bio-socio-psycho-environmental aspects.

In 2021 the biological and inflammation targeted approach (Line 1) and the methodology and behavior targeted approach (Line 2) will be combined and tested in human Proof of Concept (hPoC) study that will be conducted in 2021. The activities in 2020 in Line 2 revolved around the preparations for this study, focusing on four key parts to support the hPoC study :

1. Development of a model that will predict the best personal intervention for participants. This model will be developed by a combined use of biological and behavioral data from the Lifelines cohort. To use this, the data of the Lifelines cohort should be captured in ontologies.
2. Definition and ontologization of the outcome measures. The outcome measures are a combination of vitals and Patient Recorded Outcome Measures (PROMs) and will be targeted at metabolic syndrome MetS. The foundation for the outcome measures will be via The International Consortium of Health Outcomes Measurement (ICHOM) for diabetes or the 360ºC diagnostic tools (or a smart combination of the two).
3. Adaptation and application of Distillation and Matching behavioral model (D&M model 2.0) that will guide the participants to the correct behavioral intervention.
4. Testing and application of the ‘social contract’ framework to the hPoC study.

Results realized

Line 1: Biology

No.	Results planned	Realization
1.1.1	Differential and shared underlying pathways of lifestyle interventions	Yes
1.1.2	mPOC study samples measured for biomarker panel	Yes
1.2.1	List of validated markers from SBI	Yes
1.2.2	Lead interventions based on SBI knowledge	Yes, targets identified from SBI network were used to identify ingredients for interventions in task 1.3
1.3.1	Alternative interventions TargetTri	Yes
1.4.1	Lead interventions validated in my-screen	No, postponed to Q1/2 2021
1.4.2	Protocol for analyzing role microbiome/mycobiome In relation to human health and inflammation	Yes, this has been included in the hPOC protocol
1.5.1	Protocol for MEC submission for proof of principle study in 2021	Yes, protocol approved
1.5.2	Defined PhenFlex based innovative biomarker panel	Yes, included in METC protocol of hPOC
1.5.3	Defined fasting based innovative biomarker panel	Yes, included in METC protocol of hPOC
1.5.4	Biobank samples measured for intervention effect on (tissue specific) inflammation (biomarker panel)	Yes, Nutritech and BellyFat biobank samples were analysed to quantify intervention effect
	Reports, papers, presentations planned	
1.1	Draft manuscript of mouse POC study	Yes, data of PPS Muscle health will be added and manuscript will then be submitted in Q1 2021
1.2	Manuscript SBI for biomarker identification	Yes, first draft of manuscript is ready. It is planned to have it submitted in April 2021 to Frontiers of Physiology (issue: “Integrative Approaches to the Molecular Physiology of Inflammation”)
1.5	Manuscript on composite biomarker of inflammatory resilience	No, is partly dependent on meta-data from BellyFat study that we did not receive yet. This is planned for 2021 in collaboration with PPS PhenFlex-2 project. We may also want to consider to also include hPOC study results in this manuscript.

Line 2: Research Methodology Innovation

No.	Results planned	Realization
2a.1	A report on the crucial items that should become part of the PHAS building blocks	Yes. D2a.1tm4
2a.2	A set of building blocks for personal diagnosis	
2a.3	A set of building blocks for personal interventions	
2a.4	A set of building blocks for quantification of outcomes	
2a.5	A predictive model based on the Lifelines data	No. D2a.5 gives overview of use of Lifelines data.
2a.6	A hybrid model developed together with ERP hybrid AI on the Lifelines data	No.
2b.1	Publication on technology acceptance of the individual advice system for DM2 patients (based on the work of 2019)	Yes. D2b.1
2b.2	Updated DM model 2.0, that will be made available as interactive eTool	No, partly (PHAS).
2b.3	Proof of concept of N-of-1 trial for personalized behavior interventions	Prolonged into 2021
2c.1	Scientific paper about global health data sharing policies	Yes. D2c.1
2c.2	Master thesis about data sharing from a citizens/patients' perspective	Yes. D2c.2
2c.3	Workshop report about ethical challenges around data driven health approaches	Prolonged into 2021
2c.4	Report that describes the social contract (between patients (data donors) and data processors (researchers) that serves as a framework for FAIR-trade of personal health data	Yes. D2c.4
2c.5	Report that describes the barriers and challenges and the possibilities of scaling a practical health data marketplace	No. Transferred to project "je data de baas"
	Reports, papers, presentations planned	
1	A report on the crucial items that should become part of the PHAS building blocks	D2a.1-4
2	Scientific paper about global health data sharing policies	D2c.1
3	Master thesis about data sharing from a citizens/patients' perspective	D2c.2
4	Report that describes the social contract (between patients (data donors) and data processors (researchers) that serves as a framework for FAIR-trade of personal health data	D2c.4
5	Report that describes the barriers and challenges and the possibilities of scaling a practical health data marketplace	D2c.5 (excl)

Realized contribution to new knowledge and technology

Line 1: Biology
Mouse POC study

Results of the proof of concept mouse study provided important knowledge and first proof for the assumption that lifestyle interventions can reverse chronic inflammation and other obesity related pathologies. Furthermore, as organ specific results were obtained, the study showed that with respect to reversal of inflammation the effects were tissue and intervention specific. The additive effects of lifestyle interventions for some but not all analysed characteristics in liver, adipose tissue and muscle, provided important mechanistical clues on differential or shared underlying pathways.

Systems Biomarker Intelligence

The results of the in silico biomarker prediction approach (SBI) contributed to the development of new technology and new knowledge. New technology since the results reported here demonstrate, for the first time, a verification and validation of mechanism-based predicted biomarkers from the SBI-tool in experimental data. For this, we used transcriptome data from one mouse study (POC-study) and plasma protein data from one human (Foodmix) study.

This contributes to new knowledge since we have identified a new set of biomarkers that potentially can reflect the inflammatory status in liver and/or adipose tissue. These results are documented in a manuscript that will be submitted to Frontiers of Physiology, issue: *Integrative Approaches to the Molecular Physiology of Inflammation.*

Ultimate human study and biomarkers

Results of the biobank samples have shown that differences in inflammatory resilience by means of analyzing the PhenFlex challenge response can be detected between health and diseased, but also between young and old and different levels of adiposity. Differences in inflammatory resilience by lifestyle interventions can also be detected. Earlier we have shown that whole grain wheat can improve inflammatory resilience (Hoevenaars et al. J Nutr. 2019;149(12):2133-2144) and also first indications show that weight loss also improves inflammatory resilience especially in persons with high levels of intra-organ fat. Inflammation and inflammatory resilience and quantification of intervention effects on inflammation contributes to an improved technology position for TNO. Inflammation is an overarching process very important in health and disease and also in relation to e.g. covid-19 this is an important topic.

Line 2: Research Methodology Innovation

The TNO assets are better reusable for personalized diagnosis and interventions by the modular development of PHAS. We have a better insight in the hybrid modelling used in the health domain and have plans how to develop a hybrid models for T2D to improve the personalized intervention for individuals and prevent disease development. TNO has gained more knowledge about data sharing policies, legal requirements and governance rules in health care and for the common good.

The N=1 study has paid off: based on the study we have already gained funding via the MLDS foundation, with regard to liver fatty disease, and the acquired project is seen as a corner stone for the integration of two other funded studies.

The technological position of TNO has become stronger because the knowledge is more easily implemental in innovations of partners. For VWS the modular PHAS system can help in fulfilling the prevention goals of the department. We see an increasing demand of projects that need knowledge about the legal boundaries and governance of data sharing policies. Especially from pharmaceutical companies.

Realized contribution to the market position

The ERP aimed at developing new PPS projects in the future with a new focus on studying inflammatory resilience and how to improve this. We expect to start the first PPS in 2022.

Companies can use the TNO diagnosis and intervention knowledge and solution more easily in their products.

The developments in Line 2 have landed in the different product market combinations (PMCs) of the roadmap Digital Health (DHT), for example the use of the modular PHAS has been implemented in a demo in PMC4 of DHT. The outcomes have also landed in the PPS Connect2HealthConsumer.

Publicity

Presentations

- Inflammatory resilience: The ‘ wetenschappelijke notitie’ on inflammatory resilience and lifestyle was a.o. presented by Suzan Wopereis to Paul Blokhuis (23 June 2020 via WebEx)

Publications

Line 1: Biology

- “Wetenschappelijke notitie over de relaties tussen COVID-19, metabole ontregeling, weerstand en leefstijlinterventies”
  https://www.tno.nl/nl/over-tno/nieuws/2020/5/covid-19-maakt-duidelijk-leefstijl-en-leefstijlgeneeskunde/
  dr. Ben van Ommen (TNO), prof. dr. Hanno Pijl (LUMC), **dr. Suzan Wopereis (TNO)**, prof. dr. Jessica Kiefte-de Jong (LUMC); prof. dr. Niels Chavannes (LUMC); dr. Bas Kremer (TNO); dr. Jolanda van Bilsen (TNO); drs. Martijn van Winkelhof (Lifestyle4Health).
- Next generation health claims based on resilience: the example of whole grain wheat. Hoevenaars FPM, van der Kamp JW, van den Brink W, **Wopereis S**. Nutrients. 2020;12(10):E2945.
- From lifespan to healthspan: the role of nutrition in healthy ageing. Wickramasinghe, K., Mathers, J., Wopereis, S., Marsman, D., & Griffiths, J. Journal of Nutritional Science. 2020; 9, E33.
- Measuring health promotion: translating science into policy. Griffiths JC, De Vries J, McBurney MI, **Wopereis S**, Serttas S, Marsman DS. Eur J Nutr. 2020;59(Suppl 2):11-23.
- Current and Future Nutritional Strategies to Modulate Inflammatory Dynamics in Metabolic Disorders. van den Brink W, van Bilsen J, Salic K, Hoevenaars FPM, Verschuren L, Kleemann R, Bouwman J, Ronnett GV, van Ommen B, and **Wopereis S**. Front Nutr. 2019;6:129

Line 2: Research Methodology Innovation

- Report: Gezond gebruik van gezondheidsdata (TNO 2020 R11735)
- Report: Legal boundary conditions for processing personal health data (TNO 2020 R11763)
- Paper: Harekeh et al.. Predictors of the Acceptance of an eCoach targeting Self-management of Type 2 Diabetes Patients: A Web-Based Survey *submitted*
- Paper: M. van Lieshout, Y. vnan Gastel and A. Boorsma. Data Sharing Policies in Health Research – From individual autonomy to collective decision making. *submitted*
- Presentation: PHAS: building block definition – personal health advice systems.
- White paper on state-of-the-art of hybrid modelling in health (see ERP AI use case T2D)

Other media

- Interview Suzan Wopereis for Radar+ magazine with article entitled ‘het toverwoord weerbaarheid’ (Radar+ nr. 4, 2020, text Diana De Veld)
- Video on Lifestyle4Health website on ‘resilience and dysmetabolism (een veerkrachtig lichaam bij metabole ontregeling)
- Een veerkrachtig lichaam bij metabole ontregeling (lifestyle4health.nl)

6 ERP Organ-on-Chip

ERP Contacts: Ivana Bobeldijk (Project Lead), Evita van der Steeg/Geurt Stokman (Lead Scientist), Paulien Bongers (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

GUT-function

The objective of the ERP OoC program is to design and implement advanced human preclinical in vitro models, so called organ on-a-chip models, that better mimic human situation than current standard in vitro models do, including multiple cell types, 3D cellular architecture and combined micro-physiology to mimic body fluid flows. We will contribute to the development of stratified and/or personalized interventions by developing the concept of **population on-a-chip**. By 2023 we will develop a (stem-cell based) in vitro pre-clinical toolbox with integrated readouts, enabling the introduction of population variability earlier in drug development. This will enable development of precision medicine, support selection of drug candidates effective for specific group of patients and improve the design of clinical trial by pre-selecting patient groups already in a preclinical phase. Moreover, this will significantly reduce animal testing in preclinical development. Deliverables for 2020 will be several validation and implementation tests of specific elements of the established organ on-a-chip models (gut and liver) conducted both for pharmaceutical and nutritional applications. Integration of on-line read-out technologies of these models will continue. In addition, we will work on the connection and combination of the individual models, gut and liver, supported by mathematical modelling to translate the in-vitro results into results in humans.

Within the “gut-function-on-a-chip” program we combine biological and technical expertise and develop a predictive humanized in vitro model of the gut to study the impact of drugs, nutrition and environment on gut health. The developed model will mimic important gut characteristics, such as structure, microbiota and absorptive and secretory functions. The model will be developed by applying intestinal stem cells (isolated from human intestinal crypts) and/or human ex vivo intestinal tissue segments (InTESTine) inside novel microfluidic chips to mimic luminal and blood flow.

The developed model will be applicable for combination with microbiota derived from healthy or diseased (e.g. IBD, obese, diabetic) people in order to study (personalized) interactions between intestinal microbiota, gut epithelium and immune system in health and disease.

The developed model will have its application in the pharmaceutical and nutritional industry by providing a high physiological predictive human in vitro model to study intestinal absorption, digestion, and metabolism of compounds.

The main goal of KIP Gut 2020 was to demonstrate the added value of combining microbiota in a gut-on-chip environment, and studying populational variation in drug absorption and metabolism making use of the relevant developed gut-on-a-chip platforms.

1. Demonstrate populational variability in drug absorption and metabolism caused by differences in microbiome composition and activity (infants versus adults, healthy versus diseased) within the developed model
2. Validate the TNO gut on-a-chip model making use of human intestinal stem-cell derived organoids.
3. Develop and implement a microfluidic chip with aerobic/anaerobic interface for co-culturing of intestinal epithelial cells and human colon microbiota.
4. Proof of concept study for functional coupling kidney & gut on-a-chip, and liver & gut on-a-chip for application of prediction of first pass effect.

In the end (2021) we aim to be able to stratify patients (and their clinical responses like drug absorption, metabolism and efficacy) based on microbiome composition and activity and the interaction with gut epithelium and the immune system. Moreover, gut on-a-chip will be combined with developed liver-on-a-chip models in order to study cross-talk between organs and more accurately predict human oral bioavailability of compounds.

LIVER-function

The overall goal of the ERP OoC program is to design and implement advanced human preclinical in vitro models, so called organ on-a-chip models, that better mimic human situation than current standard in vitro models do, including multiple cell types, 3D cellular architecture and combined micro-physiology to mimic body fluid flows. We will contribute to the development of stratified and/or personalized interventions by developing the concept of **population on-a-chip**. By 2023 we aim to have developed a (stem-cell based) in vitro pre-clinical toolbox with integrated readouts, enabling the introduction of population variability earlier in drug development. This will enable development of precision medicine, support selection of drug candidates effective for specific group of patients and improve the design of clinical trial by pre-selecting patient groups already in a preclinical phase. Moreover, this will significantly reduce animal testing in preclinical development. Deliverables for 2020 were several validation and implementation tests of specific elements of the established organ on-a-chip models (gut and liver) conducted both for pharmaceutical and nutritional applications. Integration of on-line read-out technologies of these models will continue. In addition, we work on the connection and combination of the individual models, gut and liver, supported by mathematical modelling to translate the in-vitro results into results in humans.

Within the “liver-function-on-a-chip” program we will combine biological and technical expertise and develop a sophisticated, predictive, physiologically relevant (personalized) human cell-based in vitro model of NASH/fibrosis. The developed model will have its application in the pharmaceutical and nutritional industry by providing a high physiological predictive human in vitro model to study/elucidate diverse human biological processes involved in NASH/fibrosis and screen new drugs and food products which target these biological processes. By using stem cell derived hepatocytes from multiple genetically different subjects we aim to be able to stratify patients (and their clinical responses to novel pharmacologic treatments).

In 2020 we focused on the development and applications of “liver-function on a chip”. The main goal of 2020 was to further validate the 3D primary hepatocytes, stellate cells and Kupffer cells co-culture model using microfluidics (3D coculture for NASH on a chip).

- “Chip it” approach: Use of microfluidics in the current NASH/fibrosis 3D in vitro coculture model, in collaboration with KIP Technology
- Validation of the fluidics NASH/fibrosis 3D in vitro coculture model with reference compounds
- Integrate novel imaging readouts: Raman spectroscopy (for measuring levels of steatosis in spheroids), AFM (for measuring cell stiffness/flexibility), in collaboration with KIP Technology

The personalized drug development approach addressing population variability will be the focus of 2021.

- Reintroduction of stem cell derived hepatocytes in the coculture model and evaluation of effects of stem cell derived hepatocytes from multiple genetically different subjects on disease induction (including readouts via representative pathways)
- Demonstrate that the coculture model using sera of human NASH patients and human controls shows variation on disease induction in vitro (incl. readouts via representative pathways)

In the end we aim to be able to stratify patients and their clinical responses to novel pharmacologic approaches to treat NASH.

Technology

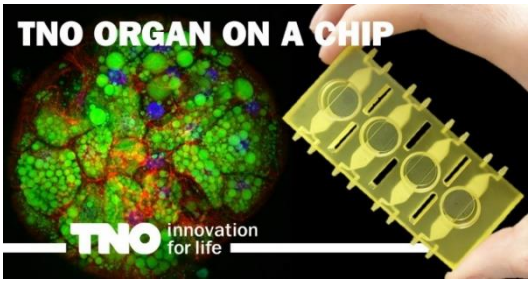

Figure 4: TNO organ on a chip

Over the past few years, the development of alternative, more physiologically relevant human cell based *in vitro* models has evolved. These so called organ function-on-a-chip models are designed to better mimic tissue function and architecture than conventional single cell based models. With these models, it will be possible to study relevant biological mechanisms and disease mechanisms. Moreover, organ function on-a-chip models provide a promising approach to solve translational issues that are evident in not only the pharmaceutical industry, but also the nutritional, chemical, environmental and cosmetic industries. The ultimate goal of organ-on-a-chip models is mimicking human (patho)physiology of specific organs within an *in vitro* system which has simple readouts. Science and in particular drug development can greatly benefit from human functional organs-on-a-chip technologies, both in terms of reliability of results and in costs.

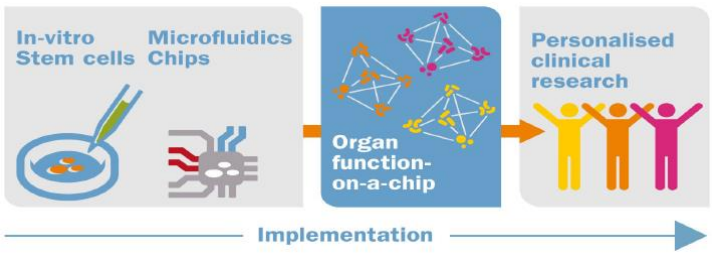

Figure 5: Implementation scheme

The challenge is to bring the models to a next level, with proven added value for science and industry: organ-on-a-chip for human diseases, long term exposure, patient-derived stem cells, providing an unique opportunity to discover personalized human drug targets, related to the underlying genetic background of the patient and to test and select the specifically designed medicines.

The overall goal of the ERP OoC program is to design and implement advanced human preclinical in vitro models, so called organ on-a-chip models, that better mimic human situation than current standard in vitro models do, including multiple cell types, 3D cellular architecture and combined micro-physiology to mimic body fluid flows. We will contribute to the development of stratified and/or personalized interventions by developing the concept of **population on-a-chip**. By 2023 we will develop a (stem-cell based) in vitro pre-clinical toolbox with integrated readouts, enabling the introduction of population variability earlier in drug development. This will enable development of precision medicine, support selection of drug candidates effective for specific group of patients and improve the design of clinical trial by pre-selecting patient groups already in a preclinical phase. Moreover, this will significantly reduce animal testing in preclinical development. Deliverables for 2020 will be several validation and implementation tests of specific elements of the established organ on-a-chip models (gut and liver) conducted both for pharmaceutical and nutritional applications. Integration of on-line read-out technologies of these models will continue. In addition, we will work on the connection and combination of the individual models, gut and liver, supported by mathematical modelling to translate the in-vitro results into results in humans.

The third research line of the ERP (Technology) focuses on the development of state-of- art organ on-a-chip hardware and (online and integrated) readout technologies, for applications within the focus use cases, but also applicable for other organs and disease areas, in collaboration with external collaborators or via licensing. In addition, we will develop specific protocols for DNA isolation from very small samples that are needed for these specific organ on-a-chip specific.

The specific objectives of this project for 2020 were:

1. Further develop and valorize the TNO designed Explant Barrier Chip and Liver chip, including relevant read-outs that the biological application (partly performed by postdoc that will be hired)
2. If feasible, Integrate the TNO chips into the TOP platform that is being developed by MESA+ at UT.
3. Develop prototype models for organ-organ interactions, including gut&liver on-a-chip and gut&kidney on-a-chip (partly through a collaboration with UMCU (postdoc))
4. Proof-of-principle for new application of sequencing technology available at TNO to study functional host-microbiome interactions in a commercially available lung model.
5. Validation of biological application of AFM technology in well-conditioned cell-culture systems for Organ-on-chip applications
6. Demonstrator for application of PBPK modelling for translating organ on-a-chip data to the in vivo situation (scaling)

Research topics:

- Can we increase throughput and easyness2use of a 3D printed microfluidic chip with a general click-in system for (intestinal) tissue, scaffolds and permeable membranes for cell culture?
- How can we ensure the compatibility/coupling of the TNO gut and liver model in the future?
- Can we add a number of simple sensors to the device for detection of TEER and gasses?
- Which readouts are the most relevant for the NASH model?
- Can we use new detection technologies such as the Nanostring technology as a relatively fast readout for advanced in-vitro systems?
- Can we analyse hepatocyte activation in spheroids?
- Can we measure mitochondrial dysfunction in vitro?
- Can we measure cellular functioning and viability online?
- Gain insight in the possibilities, limitations and uniqueness of nano-mechanical measurement techniques using current AFM systems and dedicated bio AFM systems.
- Expertise in measuring change in mechanical properties over time or due to external stimuli in a well-defined setting (e.g. by using a flow-cell)
- Develop expertise in performing reproducible and accurate AFM measurements on biological tissue with the goal to monitor the nano-mechanical properties of cells when subject to external stimuli.

Develop knowledge and expertise in the relation between the changes in tissue and the corresponding nano-mechanical properties.

Results realized

GUT-function

No.	Results planned	Realization
1	Panel of at least 10 (endogenous) biomarkers for monitoring intestinal tissue functionality and viability during 24-48 h of incubation in the InTESTine chip presented in product sheet	Yes
2	Demonstrator study showing populational variability in drug absorption, toxicity and/or epithelial immune responses to exogenous compounds making use of the InTESTine chip in combination with microbiota (supernatant).	Yes
3	Protocol for stable culturing of human ileum and colon stem-cell derived organoids, including 3D culturing, passaging and freeze-thaw cycles	Yes
4	Demonstrator study showing application of human ileum or colon stem-cell derived organoids for studying drug absorption, intestinal wall metabolism and enteroendocrine function (serotonin, satiety hormone production).	No, ongoing
5	Demonstrator study for anaerobic culturing human gut microbiota in microfluidic TNO chip for 24-48 hours	Yes, first feasibility data
6	Demonstrator study for culturing human intestinal cells in microfluidic TNO chip for 24-48 under aerobic conditions	Yes
7	Demonstrator study showing intestinal absorption and liver metabolism of at least 1 drug by applying the designed gut-liver chip	No, first feasibility experiments performed
8	Updated product sheet and ppt slides of these activities for BD purposes (continuous)	Yes
9	Publication on human InTESTine on-a-chip applications	Yes, submitted Dec 2020
10	Publication on characterization and function of personalized/populational microbiota	No, postponed to 2021
11	Oral Presentation at minimally 1 conference or workshop, 1 poster	Yes
12	Patent filing of InTESTine chip	Yes
13	Patent filing of anerobic-aerobic interface for Intestine explant barrier chip	Yes
14	Review on current intestine-on-a-chip models	Yes

LIVER-function

No.	Results planned	Realization
1	Validated protocol for the 3D model of primary human hepatocytes, primary stellate cells and Kupffer cells and its application within microfluidic chip	yes
2	Validation report of chip model system with reference compounds and respective gene expression (profiling of the model and drug effects)	Partly, transcriptome analysis in 2021
3	Slide Deck (for BD purposes) with highlights of in vitro model with primary cells, effects of reference compounds and its application within microfluidic chip	yes
4	Protocol for the 3D model of stem cell derived hepatocytes, primary stellate cells and Kupffer cells	No, planned in 2021
5	Slide Deck (for BD purposes) with results of personalized drug development approach addressing population variability	Planned in 2021
6	Report describing results of WP4	Partly
7	Report describing results of WP5	Yes
8	Grant application	TTW grant application with TU Twente, more planned in 2021
	Reports, papers, presentations planned	
1	Oral presentation at minimally 1 conference or workshop	Yes, hDMT meeting, Rotterdam, NL, 14 February EUROoCS 2020, online meeting, 8 – 9 July
2	Publication on in vitro liver co-culture model with primary cells	Planned in 2021
3	Publication of use of stem cell derived hepatocytes in in vitro liver model	No
4	At least two poster presentations at international conferences	Yes, 1 poster presentation at the Global NASH Congress, London, UK, 10 + 11 February and the same poster also at the Keystone Fibrosis meeting, UK, March 2020

Extra	Master thesis “The effect of de novo lipogenesis on NAFLD/NASH pathophysiology in in vitro models” – Elsa van der Sar	Yes

Technology

No.	Results planned	Realization
1	File patent Intestine on a chip (WP1)	*Yes*
2	First prototype Intestine-liver chip (WP1)	No, feasibility experiments (testing liver medium in intestinal models) were performed. First rough calculations of two organ systems were also done.
3	Functional working Intestine-Kidney chip (WP1)	Yes partially, the first prototype for the kidney on a chip (hollow fiber membrane) were designed and made. Detailed technical calculations to connect EBC and hollow fiber membrane chip were developed.
4	Functional working Intestine-Microbiome chip (WP1)	Yes. A conditioned chamber (patent filed) were designed and made to create aerobic-anaerobic interface on different sides of an intestinal tissue in the intestinal EBC.
5	Report on feasibility of integration of TNO chips in the UTwente TOP platform	The focus of the collaboration with Twente was integration of Liver chips. More details are described in the KIP Liver Report 2020
6	Report on experimental validation of of visco-dynamic measurements of properties of monolayer of cells (WP2)	Yes – partially. First experiments of the proof of concept are performed. Additional experiments and analysis have to be performed.
7	Plan for further development of the visco-dynamic model with industrial partners	No – experiments were delayed and the outcome is essential to perform next steps.
8	First prototype of multipurpose microfluidic chip with integrated sensors for TEER, O2 and 1 other biomarker (WP3)	Yes, TEER, oxygen, pH and glucose
9	PPP plan TNO-LUMC-Emulate-GSK (WP4)	No, Due to Covid Outbreak, the focus for GSK shifted and also the focus of TNO shifted to Covid-related activities.
10	Proof of principle study for high sensitivity sequencing of microbiota in host-microbiome interactions lung on a chip (WP4)	No, see above. All activities, including the budget have been shifted to 2021
11	Adjusted design of the gut chip to fit on the TOP platform	No, this will come after adaptation of the TOP platform on the liver on a chip.
12	Adjusted design of the liver chip to fit on the TOP platform	Yes, reported in more detail in KIP Liver report.
13	First version of algorithm to translate OoC results (gut) to human data	Yes
Extra	Patent application filed for the aerobic/anaerobic interface	Yes
	Reports, papers, presentations planned	
1	First draft paper Intestine on a chip – technological perspective	Yes, first draft has been made which will be submitted by the end of 2020 or beginning of 2021
2	First draft Review paper Intestine-Liver-Kidney on a chip	Yes, two review papers were written. One a review about intestine on a chip (Donkers et al., current opinion in toxicology) and one review about gut-kidney axis in collaboration with UU (Trends in Biotechnology)
3	First draft paper Intestine-microbiome chip	No, this will be part of KIP Darm in 2021. Most focus were spent on the practical side of the aerobic-anaerobic interface and the other manuscript.
4	Oral Presentation AFM bio-application during conference or workshop	No – no data available at Q1-2020 and conference is rescheduled to 2021.
5	2 posters or oral presentations at conferences	- Poster presentation EUROoCs 2020 - Oral presentation EUROoCS 2020 - Oral presentation SelectBio 2020 - Poster presentation AAPS Pharmsci360
6	1 manuscript Intestine on a chip	Yes partially, combined with #1. The paper will be submitted by the end of 2020 or beginning of 2021.

Realized contribution to new knowledge and technology

GUT-function

The research performed in this project has resulted in development of new knowledge and technology within TNO which has already proven to be very interesting for pharmaceutical and food industry. We are currently fully exploring the opportunities how to exploit this knowledge and technology in grants and in commercial projects

The research performed highly adds to the governmental statement “Nederland wereldleider proefdiervrije innovaties”, since we are developing game-changing animal-free preclinical models by in applying human stem cells and redundant human tissue. Moreover this work will add to improved and faster drug development which will result in better disease control and new medications for (chronic) diseases, one of the new missions of the Dutch Government.

The current fundamental and technological knowledge enables TNO to develop innovative technology in the next coming years.

LIVER-function

In 2020 we have further validated the 3D co-culture model under static and microfluidic conditions. The model seems to reflect the human biology of NASH and fibrosis. When using Emiracasan or Elafibranor in the model; compounds that failed in phase 3 clinical trials, we observed a similar outcome; no effect on fibrosis. However, when combining 3 clinical relevant compounds, fibrosis was beneficially affected in the in vitro model.

NASH is becoming a huge health problem. In addition to animal models for preclinical research the need grows (both in industry as society) for better predictive in vitro models. TNO is known for its quality and its knowledge on disease processes and translating this into predictive models. This project fits within the core of these issues, and strengthens the knowledge of TNO and the role it takes in preclinical research focusing on application and translation to the patient.

This project fits well with the 3R policy, in the future it will contribute to a more effective drug development and enable personalized medicine.

Technology

A conditioned chamber to create a double interface in perfused systems, e.g. the aerobic-anaerobic interface in the gut

Together with a dedicated technology focused team we have improved both liver and InTESTine chip systems. Integration with (online) read-out sensors has been achieved. Together with the developments in the KIP Gut and KIP Liver projects, the technology developed created a unique position for TNO, especially within hDMT.

The current fundamental and technological knowledge enables TNO to develop innovative technology in the next coming years.

Realized contribution to the market position

GUT-function

The developed organ on-a-chip technology is implemented in projects and already applied in some B2B projects (Chugai, Evonik, Ono pharmaceuticals (lead phase)) and private-public-partnerships (NoSoClo).

Our developed biology and technology enables us to participate in consortia for different grant proposals, such as NWA calls and EU proposals. Additionally, several grant projects have been submitted and some honored (as described above). All our results are regularly presented on conferences with industry participation and slides have been made and presented to several pharma and food companies. This is done focused on the intended use of the technology (gut on a chip or liver on a chip) and is reported in those projects.

Our new chip design is now described in a patent filing documents and patent will be filed next year.

The results of this project are disseminated also to the Healthy Living Roadmaps and PMC’s.

LIVER-function

In vitro NASH efficacy studies predictive for the diseased situation in patients are not available. Liver-function-on-a-chip has the potential to overcome these and other limitations of the current far-from-reality 2D in vitro assays using cell lines or in vivo models. Predictive liver-function-on-a-chip based in vitro models that represent the human situation are expected to lead to better selection of success or failure of compounds in the clinical development phase. These predictive models are a high unmet need of pharmaceutical industry, and will also be of great use to nutritional industry, which increasingly use pharmaceutical research models for testing compounds and understanding disease mechanisms. By being able to generate new predictive, physiological models, we will greatly improve the position of TNO as a knowledge and technology partner who can offer a complete portfolio regarding biological questions coming from all types of industries.

Next to poster and oral presentations on different congresses a TKI with stichting proefdiervrij and Galapagos has been continued in 2020. Different presentations have been given to pharmaceutical and biotechnology companies, e.g. NordicBiosciences etc.

It is expected that development of new technologies/applications such as foreseen in this project can be protected. Throughout the project, results will therefore be carefully monitored and options for patenting will, when relevant, be explored.

Technology

The technology developed within this project can be applied in organ on a chip models developed and offered by TNO, gut and Liver. However the technology (Chips, Anaerobic chamber) can be valuable also for other applications. A market-possibility brainstorm was organized in Q1, when the different possibilities were discussed (attendees were scientists and business developers). Different ideas were listed and where possible, first contacts were made (see below).

The following actions for commercialization of the results have been initiated:

- Meetings for collaborations with Uppsala university to have them test the intestinal EBC
- Meetings for collaborations with VUMC Amsterdam to have them test the skin EBC
- Meetings for collaborations with MatTek to use the first prototypes of cell applications of the EBC
- All of the above to enable commercializations in different areas of application (outside of TNO).
- Within TNO, the developed chip and the technology for applications gut model and liver model, these have been presented to different industrial partners that are interested in testing the safety or efficacy of different (drug) interventions. The companies are listed in the individual report of Liver and Gut projects.
- The Explant Barrier Chip (EBC) and the Anaerobic chamber were filed for patent

Publicity

General

Publications

- Several LinkedIn posts
- Ostendorf R, Development of a diet-induced disease-mimicking in vitro model of non-alcoholic steatohepatitis (NASH)/ fibrosis, poster 3rd Global NASH Congress, London, UK: – February 2020
- Bobeldijk I, Organ on a chip @TNO, Presentation at the opening of the Organ on a chip Centre, Twente, October 2020

GUT-function

Publications

- Donkers J.M. Modeling host-microbe interactions in the InTESTine Barrier Chip using human ex vivo intestinal tissue. EUROoCS 8-9 July 2020, oral presentation
- Eslami Amirabadi H, InTESTine Barrier Chip: A medium throughput microfluidic system to study barrier functions. EUROoCS 8-9 July 2020, poster presentation
- Eslami Amirabadi H, InTESTine Chip: a microfluidic ex vivo model to study intestinal permeability and host-microbe interactions in the human intestinal tract. SelectBio 9-10 sept 2020, oral presentation
- Donkers J.M. InTESTine Barrier Chip: a medium throughput microfluidic system to study drug absorption and host-microbe interactions in ex vivo intestinal tissue. AAPS Pharmsci360 26 okt-5 nov 2020, poster presentation

- Langerak N, Ahmed HMM, Li Y, Middel IR, Eslami Amirabadi H, Malda J, Masereeuw R, van Roij R. A Theoretical and Experimental Study to Optimize Cell Differentiation in a Novel Intestinal Chip. Front Bioeng Biotechnol. 2020 Jul 24;8:763., manuscript
- Donkers J.M. Intestine-on-a-chip: next level *in vitro* research model of the human intestine. Current opinion in Toxicology, online 4 dec 2020, manuscript
- Cahier (issue of the Dutch life sciences and society foundation) "Mini organs on chips", with contributions from Geurt Stokman, Roeland Hanemaaijer and Evita van de Steeg, who show the latest developments in the field of in vitro research models for disease and treatment with liver-on-a-chip and intestine-on-a-chip. In collaboration with hDMT

Evita van de Steeg – since December 2020 chair of the Gut-Liver on-a-chip (GLoC) theme group of hDMT, responsible for organizing scientific theme group meetings - chair

IP: Patent publications etc.

- Donkers J.M., Eslami Amirabadi H. Sealing chamber for dual-interface fluidic system. Patent filed: TNO ref: 2020030 HL/BH # 51051011 (V.O. ref: P127612EP00). Sept 2020.

LIVER-function

Poster presentations:

- Ostendorf R, Development of a diet-induced disease-mimicking in vitro model of non-alcoholic steatohepatitis (NASH)/ fibrosis 3rd Global NASH Congress, London, UK: – February 2020
- Hanemaaijer R, Development of a diet-induced disease-mimicking in vitro model of non-alcoholic steatohepatitis (NASH)/ fibrosis, Keystone Fibrosis symposium, US, March 2020

The Gut-liver on a chip meeting to be hosted by TNO and hDTM was cancelled mid-March because of Covid-19.

Oral presentations:

- Ahmed H, In vitro disease modelling using a novel organotypic 3D culture, hDMT meeting, Rotterdam, NL: February 2020
- Ahmed H, Development of a diet-induced model for NASH and fibrosis in a spheroid-based liver-on-chip model, EUROoCS 2020, online meeting: July 2020

Publication in Cahier (issue of the Dutch life sciences and society foundation) "Mini organs on chips", with contributions from Geurt Stokman and Roeland Hanemaaijer, who showed the latest developments in the field of in vitro research models for disease and treatment with liver-on-a-chip. November 2020.

Technology

Publications

- Laura Giordano, Silvia M. Mihaila, Hossein Eslami Amirabadi, Rosalinde Masereeuw, “MICROPHYSIOLOGICAL SYSTEMS TO RECAPITULATE THE GUT-KIDNEY AXIS”, Trends in Biotechology (2020), in press
- Donkers J.M. Modeling host-microbe interactions in the InTESTine Barrier Chip using human ex vivo intestinal tissue. EUROoCS 8-9 July 2020, oral presentation
- Eslami Amirabadi H, InTESTine Barrier Chip: A medium throughput microfluidic system to study barrier functions. EUROoCS 8-9 July 2020, poster presentation
- Eslami Amirabadi H, InTESTine Chip: a microfluidic ex vivo model to study intestinal permeability and host-microbe interactions in the human intestinal tract. SelectBio 9-10 sept 2020, oral presentation
- Donkers J.M. InTESTine Barrier Chip: a medium throughput microfluidic system to study drug absorption and host-microbe interactions in ex vivo intestinal tissue. AAPS Pharmsci360 26 okt-5 nov 2020, poster presentation
- Langerak N, Ahmed HMM, Li Y, Middel IR, Eslami Amirabadi H, Malda J, Masereeuw R, van Roij R. A Theoretical and Experimental Study to Optimize Cell Differentiation in a Novel Intestinal Chip. Front Bioeng Biotechnol. 2020 Jul 24;8:763., manuscript
- Donkers J.M. Intestine-on-a-chip: next level *in vitro* research model of the human intestine. Current opinion in Toxicology, online 4 dec 2020, manuscript
- Paul Vrenken, Master Thesis

Further: patent descriptions, premier depots.

- Patent application filed: MICROFLUIDIC DEVICE FOR ANALYZING A MEMBRANE (Explant Barrier Chip)
- Patent application filed: CONDITIONING CHAMBER FOR DUAL-INTERFACE FLUIDIC SYSTEMS (Anaerobic chamber)

7 ERP Submicron Composites

ERP Contacts: Aike Wypkema (Project Lead), Pascal Buskens (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

The overall goal of this ERP is to achieve a level of control over structure and chemical composition of materials that enables the development of materials with programmable functionality. Furthermore, we aim to progress from state of the art monofunctional materials via materials with multiple passive functionalities to active and adaptive materials. We will demonstrate the knowledge gained within the framework of this ERP in selected use cases chosen in collaboration with the Brightlands Materials Center and its partners.

The research within this ERP supports activities of the Brightlands Materials Center (BMC). In collaboration with other partners in BMC, we will select use cases which are of relevance for the following BMC programs:

- Additive manufacturing (AM)
- Sustainable Buildings (SB)

The ERP will achieve its ambition by developing a systematic approach connecting relevant numerical (modelling) and experimental (synthesis, analysis, and characterization) methodologies.

Additive Manufacturing

In 2020, we aimed to achieve the following:

A. 3D printed parts for high mechanical load and structural integrity monitoring:
   - Material and process development will be focused on using continuous carbon fiber for mechanical reinforcement, and optimizing process conditions to achieve a stiffness of 50 GPa and a strength of 260 MPa, which would allow replacement of metal products leading to significant weight reduction.
   - Concept and manufacturing of 3D printed sensors embedded in filament deposition modeling. After the first proof of principle, sensing within continuous filament printing needs a boost to make a leap forward towards applications in structural integrity monitoring or heat management. The current issue lies largely within the selectivity of the active sensing element and also its responsiveness. We aim at determining the right material combination (filament plus fiber) as well as configuration for the manufacturing of device-/material-integrated strain and pressure sensors.

B. Incorporate stimuli-responsive functionality during printing:
   - Demonstrate the use of resins based on liquid crystalline building blocks or containing micro- and nanoparticles for the manufacturing of an active sensor within a 3D printed part. The functionality enabling the sensor is due to the alignment of the liquid crystals or microparticles and its response after it is subjected to an external stimulus. This work will be a further implementation of the results of PhD projects performed at TU/e in the domain of photocurable resins.

Sustainable Buildings

The overall goal is to develop nanocomposite glass coatings and polymer nanocomposite films for glass lamination, to improve the energy efficiency of buildings.

In line with the BMC program Sustainable Buildings, we selected infrared regulating polymer films and coatings, and coatings or materials that capture light on large surface areas and guide it to a position where it can be used e.g. in combination with photovoltaic modules. Both materials have the potential to contribute to improving the energy efficiency of buildings, which is highly relevant in view of European, national and regional ambitions regarding energy neutrality in the built environment. To achieve the required functionalities, we will design and synthesize functional nanomaterials, and disperse those in polymer matrix materials in a controlled fashion. The infrared regulating polymer films are an illustrative example of a material with a dynamic functionality; they will be adaptive in response to temperature.

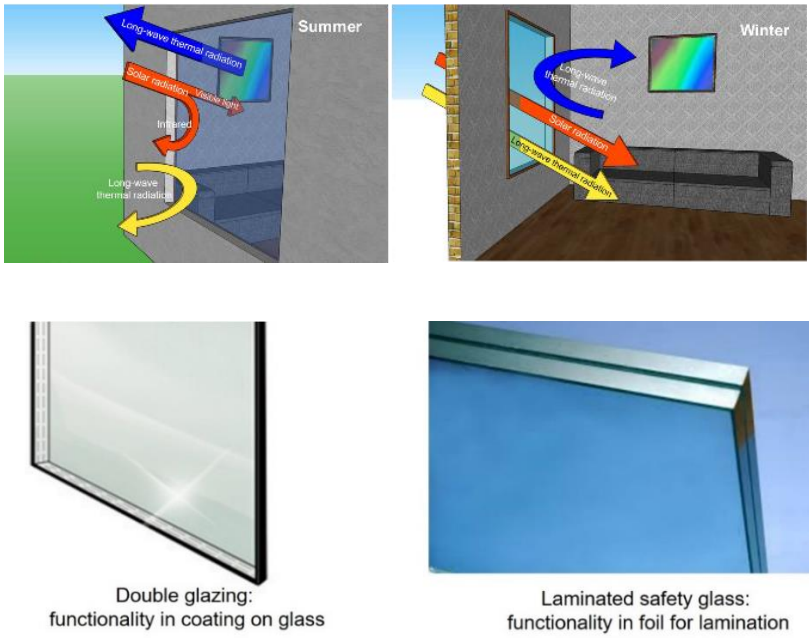

Figure 6: Thermochromic glass coatings and polymer films for thermochromic heat regulating windows

Focus of the ERP until 2021 is on thermochromic nanocomposite coatings and films, that can switch from solar heat transmission to blocking and vice versa at a specific temperature. Such coatings/films outperform the current state of the art products, i.e. low-E coatings and static heat-reflective films, by up to 30% with respect to energy savings for heating and cooling of buildings. Ergo, this significantly contributes to realizing the sustainable energy and climate targets, specifically for the built environment.

Results realized

Additive Manufacturing

No.	Results planned	Realization
1	Proof of concept of mechanical strength (260 MPa) in simple test geometries	Yes. Strength of 600 MPa reached which has surpassed the initially intended value.
2	Report comparing the economics of producing fiber-reinforced 3D printed parts with metal parts or composites parts produced by other methods	Yes. The report has been delivered.
3	Implementation of developed processing strategies in complex 3D demonstrator to achieve same mechanical strength	Yes. Performance in non-trivial geometries obtained. Examples are connecting rods, bike lugs. Characterization of the strength in 3D is still in progress (Nov 2020), in collaboration with 100% Limburg Bike project.
4	Implementation of modelling workflow for continuous fiber AM	Yes. Modeling workflow has been implemented.
5	Demonstrator of integrated strain sensing correlated with internal microstructure variations	Yes. Several demonstrators have been realized. They emphasize on multi-sensing, localization and user loading response.
6	Demonstrated functionality of 3D part based on particle alignment during printing	No. The lack of a user case of commercial relevance was the main reason.
7	Patent application(s) regarding particle alignment during printing and/or integrated sensing	Yes. Two patents have been submitted (sensing and particle alignment). Current status is pending patentability.
	Reports, papers, presentations planned	
1	Conference presentation at JEC fair	Not possible. Event cancelled due to COVID-19
2	Conference presentation at LOPEC	No. Vide supra.

Sustainable Buildings

No.	Results planned	Realization
1	Thermochromic VO2 particles with a particle size less than 5 µm, obtained via bottom up synthesis	Yes, vide supra
2	First lab-scale batch of thermochromic nanoparticles with a particle size below 100 nm, and a switching enthalpy ≥ 20 J/g prepared	Yes, vide supra
3	Surface functionalized VO2 particles with a particle size less than 100 nm, obtained via top-down synthesis	Yes, vide supra
4	Thermochromic nanocomposite PVB film comprising thermochromic nanoparticles yielding an additional reduction in energy consumption over the single layer coating of at least 5%, to be demonstrated using EnergyPlus modeling.	No, we prepared first films which were not yet of sufficient quality to quantify their thermochromic performance as glass interlayer, vide supra
5	First 3-layer thermochromic coating stack prepared on 10x10 cm^2 glass samples	No, we have not pursued multilayer coatings since our single layer coating outperforms state of the art systems, vide supra
6	Multi-layer thermochromic coating stack with improved properties over BMC single-layer system, yielding an additional reduction in energy consumption over the single layer coating of at least 5%, to be demonstrated using EnergyPlus modeling.	No, we have not pursued multilayer coatings since our single layer coating outperforms state of the art systems, vide supra
	Reports, papers, presentations planned	
1	1 scientific publication on thermochromic powders/nanoparticles/coatings (together with UHasselt)	Yes, 2 published, 2 submitted, vide infra. Furthermore, 2 new patent applications filed.
2	At least 3 contributions to (inter-)national symposia and conferences	No, due to pandemic related cancellations only 2 contributions were possible, vide infra

Realized contribution to new knowledge and technology

Additive Manufacturing

The project has strengthened the technology position of TNO in the field of continuous fiber additive manufacturing. The results from WP1 and WP2 have strongly increased our knowledge in the relation between processing conditions, product microstructure and mechanical performance. In combination with the results of WP3 we have gained more understanding on the design and fiber lay-out for 3D printed parts. The result in the technical steps from WP4 have helped to close the gap needed to offer self-sensing for strain and load monitoring to parties interested. With the help of the current patent the position of TNO can be boosted in domains where continuous monitoring of the primary function of composite parts is required.

Sustainable Buildings

New knowledge and technology has been acquainted in:

- Solution processed thermochromic VO_2 coatings
- Synthesis of thermochromic VO_2 pigments
- Integration of thermochromic VO_2 pigments in polymers such as PVB to produce nanocomposite films using extrusion
- Characterization of thermochromic coatings and polymer films

The ERP strengthens the technology position of the BMC-TNO program Sustainable Buildings, in which thermochromic coatings and films are a major focus area as technologies to reduce the energy consumption for heating and cooling of buildings.

The ERP contributes to reducing energy consumption and CO_2 emission in the built environment. Major partner companies for these technologies are pigment producers (e.g. Kriya, Ferro, BASF) and polymer film producers (e.g. Sekisui, Everlam, Sabic, Yparex). However, we focus on mobilizing the entire customer value chain from materials producer to end user.

Realized contribution to the market position

Additive Manufacturing

Despite the lack of events this year our self-sensing technology has awaken the interest of several parties. This year we started to formulate a project to realize a smart gasket together with Sitech. In this project a pipe sealing device was to be developed in order to certify the procedure during installation or replacement of parts, therefore saving maintenance cost. The first proposal was submitted and amounted to a value of 35kE.

In addition we have started contact in the field of wearable robotics where lightweight embedded sensors are required. In a similar fashion that feature is needed in the making of self-steering drones. They will be used to provide feedback on the status of their wings. In doing so it will be possible for the drone's system to learn maneuver and adapt in different weather conditions.

Regarding the mechanical performance of CFAM products, discussion on follow-up projects are ongoing with GKN Aerospace Fokker, SGL Carbon, Anisoprint, Viro, Ensinger and Futura Composites.

In 2020, two patent applications were filed on the developed technology.

Sustainable Buildings

This project provides new basic knowledge for TNO/BMC, which forms the basis for the foreseen increase:

- in the number of partners in the BMC Shared Research Program (1-2 new partners per year);
- in the turnover of the program Sustainable Buildings (ca. from 1.5 Mio € to 2.5 Mio € per year).

Realization: The ERP Submicron Composites project enabled us to start the TKI project THERPA, the Interreg Flanders-Nederland project SUNOVATE and the OPZuid project LEEF. Adding 8 new partners to the BMC Shared Research Program and realizing an order intake for the Sustainable Buildings program of 3.0 Mio €.

The know-how that will be gathered within this ERP will be very important to acquire new partners for BMC's Sustainable Buildings shared research program. We will primarily target glass producers (e.g. AGC, Saint-Gobain, Guardian, NSG) for the thermochromic coating development, and polymer/film producers (focus on PVB, e.g. Sekisui, Everlam, Eastman) for the nanocomposite thermochromic film development.

Realization: We started 3 new projects with industry partners to scale up our technologies to move further towards commercialization. Furthermore several new EU and Interreg proposals and bilateral projects with industry partners are in preparation. Additionally we have started an investigation into the possibility to start a tech transfer for the thermochromic single layer coating.

At least one new patent application was foreseen in 2020. One existing patent application was substantially strengthened and two new patent applications were realized in 2020

Publicity

Additive Manufacturing

- New developments of short and continuous fiber printing with exceptional mechanical behavior and unique functionalities. RapidPro, Conference, Veldhoven (NL) 05-03-2020 (César Stüpp).
- Additive Manufacturing with Continuous Fibers. CompositesNL - Sustainability in Composites, webinar, 23-06-2020 (Richard Janssen).
- Continuous fibre printing with exceptional mechanical behaviour and unique functionalities. Next Level 3D Printing, Webinar organized by BMC, 25-06-2020 (César Stüpp).
- Optimization and monitoring of mechanical performance of 3D printed fiber reinforced products. SAMPE Europe Conference, Amsterdam (NL), 30-09-2020 (Tessa ten Cate).
- Performance and calibration of continuous carbon fiber sensing in 3D printed parts (Journal of Sensor Technology, in prep. Fidel Valega).
- Supporting industrial innovation with R&D in Continuous Fiber Additive Manufacturing (Tessa ten Cate, Richard Janssen, ITHEC, 15-10-2020).
- Added functionality within additive manufactured products (Fidel Valega, 26-03-2020, LOPEC 2020 Scientific Conference; last minute cancellation due to COVID-19).

Remark: JEC 2020 and other exhibitions canceled due to COVID-19. Formnext 2020 is still scheduled to take place in Nov. 2020.

Sustainable Buildings

- Mann et al., Energies 2020, 13, 2842.
- Waulthers et al., Polymers 2020, 12, 1557.
- Calvi et al., JSolar Energy Materials & Solar Cells 2020, submitted.
- Yeung et al., Sol. Eng. Mater. Sol. Cells 2020, submitted.
- Presentation at EU PVSec, virtual conference, September 2020.
- Presentation at glasstec virtual, virtual conference, October 2020.
- Radio interview at NPO 1.

Patent descriptions, premier depots.

PLT#	**Title**
2018151	Thermochromic Nanocomposite Coatings
2020042	Advanced Thermochromic Coatings (2-step cure)
2020056	Monoclinic VO2

8 ERP i-Botics

ERP Contacts: Heather Young (Project Lead), Jan van Erp (Lead Scientist), Hajee van Veen (Science Director)
ERP Duration: 2018 – 2021

Progress 2020

Objectives

The Joint Innovation Centre (JIC) i-Botics (founding partners TNO and the University of Twente (UT)) formulated a Technology Roadmap (TNO-2016-R11705), that includes the strategic objectives for the ERP. On September 17th, 2018, the JIC partners TNO and UT recalibrated this roadmap, resulting in a sharpening at detailed levels. In October 2019, the JIC together with four additional partners prepared and submitted a proposal and roadmap for the ANA Avatar XPRIZE competition. The main tracks of this ERP are perfectly in line with those activities and are described below.

We (the ERP i-Botics) have the following main long-term objectives, directly related to the i-Botics Technology Roadmap):

1. To know how to realise intuitive, bimanual, dexterous remote control. We follow the telepresence approach, a combination of tele-manipulation (robot arms and hands that feel and work as one's own arms and hands), and tele-perception (3D hearing and 3D viewing at a distance).
2. To know how to create multi-sensorially enhanced control to support perceptual-motor intelligence of the operator, to enhance Situation Awareness and manipulation capabilities. This makes the robot operator more successful in task performance by using the complete range of available data of the world (e.g., user-defined, a priori, sensor and models). The focus will lie on visual sensor data, but incorporation with other sensors is also covered.
3. To develop the knowledge and technology for a wearable robot for two types of application: first, to provide mechanical support to workers who are involved in physically heavy, mobile, and 'difficult-to-automate' situations, and second, to give mechanical support to people with impaired motor functioning (elderly, sick, disabled) at home or at work. We will concentrate first on actuated exoskeletons and the underlying technology to make them effective and acceptable in realistic industrial task profiles.

The objectives of i-Botics help increase the strong position of the research groups:

- Perceptual and Cognitive Systems and Training and Performance Innovations in telepresence and bimanual haptic manipulation and feedback, for 2020 specifically on expected functional benefit of robotic ownership;
- Intelligent Autonomous Systems, for 2020 specifically on strengthening knowledge position on system engineering, in addition to remote manipulation.
- Sustainable Productivity in industrial ergonomics and wearable robotics, for 2020 specifically on tuning of active exoskeletons and applications to arm motion support;
- Intelligent Imaging, on complex, asynchronous automated vision systems, for 2020 specifically on using multiple sensors to create operator SA (in low bandwidth conditions as well), and to extract physical object properties that can be used in task conduction and represented in virtual reality.

Strengthening these groups' excellent positions in the field of robotics is needed to remain leading and to enable TNO to continue solving customer problems regarding interactive robotics in the future. Furthermore, ERP i-Botics combines the different technologies from these research groups, making it possible to address customers' questions that these research groups would not be able to address individually.

Results realized

No.	Results planned	Realization
1	State-of-the-art bimanual tele-operated set-up	Yes, the set-up was augmented with another arm and a demo of the system was given at Eurohaptics conference.
2	Task-battery for (bimanual) teleoperations	Report on bimanual tasks is drafted. Additionally, we aim to publish the review in a scientific journal and develop a benchmark test for bimanual tele-operation performance.
3	Demonstration of complete pipeline including symbolic object representation and transfer	Yes

4	Demonstrator with active back support exoskeleton RoboMate	No. Due to COVID 19, Our partner Instituto Italiano Technologia (IIT) was not able to build our exoskeleton. However, we worked together on a lease / collaboration framework for the active back support exoskeleton. We made a list of requirements and discussed the possible control algorithms.
5	For each hackathon session: PowerPoint on challenge objective, including results/findings/followups, and dissemination pictures/videos	The hackathon as such was cancelled due to COVID 19. Instead, and interactive demo was given during Eurohaptics.
8	Eurohaptics 2020 conference	Yes.
9	All WPs: i-Botics demonstration day.	Due to COVID 19 we were unable to host a demonstration day on location.
10	Signed 'samenwerkingsovereenkomst' JIC, UT and TNO	No. The negotiations are ongoing. With Peter Werkhoven and Hajee van Veen involved.
	Reports, papers, presentations planned	
1	Publication on 2019 results (haptic feedback) prepared and submitted	Yes
2	Publication on 2020 results on haptic and visual feedback prepared and submitted [if appropriate]	Replaced by another publication. Visual aspect was not continued but instead we focused on embodiment aspects. An experiment on a potential objective marker of embodiment was conducted, data analyzed, and results reported and presented at the ICMI conference.
3	Publication on 2020 results on embodiment factors prepared and submitted [if appropriate]	Ongoing. The experiment was conducted, but data needs to be analyzed and results reported.
4	Publication on 2020 results on embodiment and task performance prepared and submitted [if appropriate]	Ongoing. The experiment was conducted, but data needs to be analyzed and results reported.
5	Paper on complete pipeline, to be submitted to IROS2020	Yes
6	Paper on MSMA SLAM model, probably journal	Ongoing. The paper is not yet submitted or approved. Writing and experiments are in progress. The total pipeline/framework is finished.
7	Journal Paper: The effectivity of a passive arm support exoskeleton in reducing muscle activation during plastering activities.	Yes: The effectivity of a passive arm support exoskeleton in reducing muscle activation during plastering activities. Ergonomics (In Press)
8	Presentation at Exo-Berlin, or Werob (Share knowledge from review 2019, and future work on active arm support exos)	Yes: Three extended abstracts were accepted for publication and presentation at WeRob (in Press): 1. The experience of plasterers towards using an arm support exoskeleton 2. Calibrating an EMG-Driven Muscle Model and Regression model to estimate moments generated actively by back muscles for controlling an actuated exoskeleton with limited data 3. Can HDEMG be used to evaluate effects of an exoskeleton on low back muscle fatigue during prolonged trunk bending? A pilot study
9	Journal Paper: Various control mechanisms of trunk support exoskeletons.	1. Yes: Evaluation of an Acceleration-based Assistive Strategy to Control a Back-support Exoskeleton for Manual Material Handling, (accepted by Wearable Technologies)
10	Human body impact of EMG based control of a trunk-support exoskeletons.	Yes: Selecting the appropriate input variables in a regression approach to estimate actively generated muscle moments around L5/S1 for exoskeleton control. (Published in Journal of Biomechanics)
11	Cooperation in ANR proposal	ANR is the French National Research Agency. The outcome of the proposal has not yet been communicated

Realized contribution to new knowledge and technology

Within the ERP i-Botics we look at the optimal human-robot interaction to perform different tasks in challenging, unpredictable and dynamic situations. We focus on direct tele-operation by humans (telepresence inspection, maintenance, …) and wearable robotics such as exosekleotons/ exosuits to enhance human capabilities.

Line Bimanual manipulation

The goal of this research line is to know how to realise intuitive, bimanual, dexterous remote control. We follow the telepresence approach, a combination of tele-manipulation (robot arms and hands that feel and work as

one's own arms and hands), and tele-perception (3D hearing and 3D viewing at a distance). This work contributes to the state of the art through innovations in the areas of performance enhancing effects, including critical and non-critical haptic cues, or (cross-modal) substitutes in remote-control tasks; factors influencing embodiment such as the conditions for embodiment of a robotic arm and how to sustain embodiment; and the relationship between embodiment and task performance.

Figure 7: TNO's bimanual setup

Line Visually enhanced control

The goal of this research line is to know how to create multi-sensorially enhanced control to support perceptual-motor intelligence of the operator, to enhance Situation Awareness and to enhance manipulation capabilities. This makes the robot operator more successful in task performance by using the complete range of available data of the world (e.g., user-defined, a priori, sensor and models). The focus lies on visual sensor data, but incorporation with other sensors is also covered. Specifically, we create a multi-sensory VR environment for situational awareness in a remote environment together with the embodied robot model that the operator controls; complete the pipeline to interpret the environment and to create symbolic object representations and their transfer to live operator VR; and apply multi-sensory data from multiple agents as a combined environment representation for the operator: MSMA-SLAM Estimate relevant object properties for robotics using visual information. Examples of relevant tasks are reading text in VR, using a stereo-camera to pick up small objects, and using the live 3D for automatic path-planning for the robot-hand or to provide a virtual top-view.

Line Exoskeleton/wearable robots

In 2020 we worked on the control of an active back support exoskeleton, the application of a passive arm support exoskeleton in realistic working tasks and a sensor based method to determine the potential of an exoskeleton in working situations. Furthermore, we made progress towards a demonstrator with a back support exoskeleton and a controller optimized for effectiveness and usability in practice.

We worked on multiple algorithms that generate a, possibly real-time, estimation of the moments in the lower back. These moment estimations can directly be linked to the optimal amount of support to be provided by an active back support exoskeleton. The first approach uses and EMG-driven biomechanical model that accurately represents the muscle mechanics in the lower back. The second approach is a regression-based model.

We created a sensor-based tool which helps determine the potential for exoskeletons in heavy work. The tool uses data from an xsens suit and obtains movement characteristics that are relevant for determining the potential of exoskeleton use during heavy work.

Realized contribution to the market position

The new knowledge on the points listed under 'progress realized', have a positive influence on the position of TNO (turnover and customers). ERP i-Botics is the driving force behind multiple projects that have been created and new projects in initiation phase. The best example is the i-Botics Avatar XPRIZE project (international competition on telepresence), which was awarded because of developments realized in this ERP. Other examples of project that have been initiated based on the ERP knowledge and market position are: RobMoSys 2.0, H2020-DT-ICT-2: RIMA, H2020 MOSES, JIP SURE, Exoskeleton Knauf project, etc.

High interest from companies and institutions, universities that is shown at different conferences is also a very positive indication. Results have been realized as much as possible in publications. Furthermore, the submission

to XPRIZE has shaped a new consortium for taking part in the competition and the project XPRIZE will give much publicity of the i-Botics work as well.

Publicity

Publications.

- A.W. de Vries, F. Krause & M.P. de Looze (2021) The effectivity of a passive arm support exoskeleton in reducing muscle activation and perceived exertion during plastering activities, Ergonomics, DOI: 10.1080/00140139.2020.1868581
- T. Kermavnar, A. W. de Vries, M. P. de Looze, and L. W. O'Sullivan, "Effects of industrial back-support exoskeletons on body loading and user experience: an updated systematic review," Ergonomics, pp. 1–48, Dec. 2020, doi: 10.1080/00140139.2020.1870162.
- A. W. de Vries, M. P. de Looze, and F. Krause, "The experience of plasterers towards using an arm support exoskeleton," 2020 Int. Symp. wearable Robot., vol. In Press, 2020.
- A. Tabasi, I. Kingma, M. P. de Looze, W. van Dijk, A. S. Koopman, and J. H. van Dieën, "Selecting the appropriate input variables in a regression approach to estimate actively generated muscle moments around L5/S1 for exoskeleton control," J. Biomech., vol. 102, p. 109650, 2020, doi: 10.1016/j.jbiomech.2020.109650.
- Maria Lazzaroni, Ali Tabasi, Stefano Toxiri, Darwin G. Caldwell, Elena De Momi, Wietse van Dijk, Michiel P. de Looze, Idsart Kingma, Jaap H. van Dieën and Jesús Ortiz (accepted by Wearable Technologies), "Evaluation of an Acceleration-based Assistive Strategy to Control a Back-support Exoskeleton for Manual Material Handling (accepted by Wearable Technologies)
- Ali Tabasi, Maria Lazzaroni, Niels P. Brouwer, Idsart Kingma, Wietse van Dijk, Michiel P. de Looze, Stefano Toxiri, Jesús Ortiz, Jaap H. van Dieën, "Calibrating an EMG-Driven Muscle Model and Regression model to estimate moments generated actively by back muscles for controlling an actuated exoskeleton with limited data.", Int. Symp. wearable Robot., vol. In Press, 2020.
- Niels Brouwer, Ali Tabasi, Alejandro Moya-Esteban, Massimo Sartori, Wietse van Dijk, Idsart Kingma and Jaap van Dieën, *"Can HDEMG be used to evaluate effects of an exoskeleton on low back muscle fatigue during prolonged trunk bending?* A pilot study.", 2020 Int. Symp. wearable Robot., vol. In Press, 2020.
- Pim Verhagen, Irene Kuling, Kaj Gijsbertse, Ivo V. Stuldreher, Krista Overvliet, Sara Falcone, Jan van Erp and Anne-Marie Brouwer. 2020. *"The Cross-modal Congruency Effect as an Objective Measure of Embodiment. In Proceedings of 2020 ACM International Conference On Multimodal Interaction"* (ICMI'20), October 25-29, Utrecht, Netherlands. ACM, New York, NY, USA, 5 pages. https://doi.org/10.1145/3395035.3425264
- Kuling I.A., Gijsbertse K., Krom B.N., van Teeffelen K.J., van Erp J.B.F. (2020), *"Haptic Feedback in a Teleoperated Box & Blocks Task."* In: Nisky I., Hartcher-O'Brien J., Wiertlewski M., Smeets J. (eds) Haptics: Science, Technology, Applications. EuroHaptics 2020. Lecture Notes in Computer Science, vol 12272. Springer, Cham. https://doi.org/10.1007/978-3-030-58147-3_11

Podcasts:

- A podcast in which Nanda van der Stap (TNO) explains everything about the intelligence and autonomy of the latest Dutch robots. Source: Hummelen, J., & van der Stap, N. (2020, 23 juni). *DE BNR TECHNIEKTOUR: DE TECHNIEK ACHTER ROBOTS. bnr.nl.* https://www.bnr.nl/podcast/techniektour/10413323/techniek-achter-robots
- Michiel de Looze was invited for a podcast on exoskeletons in collaboration with the ministry of defense in the context of Innovember. *De Ironman-suit bestaat, veel meer en veel eenvoudiger dan je denkt!* https://vimeo.com/481222369

Media appearances

- The need of tele-operated systems and the key factors of successfully deploying such systems, such as embodiment dexterity and haptic feedback was presented at the show "Universiteit van Nederland" by Irene Kulling. Our work on this topic was mentioned and illustrated.
- In a mission of the television show "Klaas kan alles" our tele-operated system was used to help escaping Klaas from a glass box Houdini-style. Additionally, the system and related research was presented on the show.

9 ERP Structural Integrity

ERP Contacts: B. Luiten (Project Lead), H. Miedema (Lead Scientist), A. Adriaanse (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

The Early Research Program Structural Integrity Digital Twin (ERP SI DT) focusses its research on a major societal issue (integrity of macro-structures) and a number of highly qualified TNO researchers from different disciplines and units are involved in this research. The major challenge of this project is to develop and effectively align building blocks for the four use cases of the ERP SI DT, tailored to the needs of prospective customers. ERP SI DT results will be communicated to the world (within TNO itself and outside of TNO), leading to joint follow-up research with other research institutes and industry, and application by stakeholders.

The ERP is subdivided in four research lines, shown in the picture below:

- Digital Twin Technologies (generic technology “toolbox”)
- Existing structures (object and component level for three use case)
- Network Vehicle Load (network level existing structures)
- Design of structures (for one use case, military vehicle made of light weight composite material)

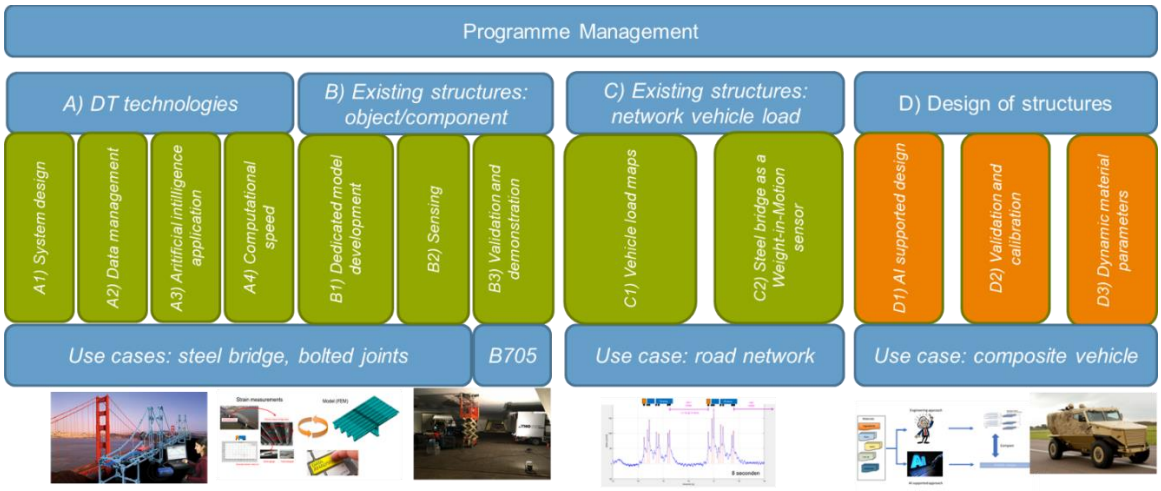

Figure 8: ERP DT SI: Overview of the Research Lines

The objectives for each research lines are next described.

Line A: Digital Twin Technologies

The general goal of research line A was to develop a system architecture that supports the requirements for digital twin for Structural Integrity assessments. This system architecture should support and incorporate the interaction between physical models, AI, Machine Learning and ontologies for data management. Besides the development of an system architecture also the implementation of this design was an important goal to demonstrate its workings. The Digital Twin platform should facilitate the position of a digital twin between the TNO-Quick scan method (a relative classification between structures) and heavy full FEM analysis to be able to deliver an absolute approximation and quantity safety in a more systematic and automized way.

Line B: Existing structures: component & structure – Modelling & Sensing

There are three long term objectives set for the use cases Steel Bridge (SB) and Offshore Wind Turbine (OWT):

B1. Model development (depicted as B1 in *Figure 8*)

We distinguish five approaches that differ in how much they rely on a physical model versus measurement data from the object:

A. Physical model only approach: Computational-based physics with prior information
B. Hybrid-physics-based data approach: using machine learning for developing a machine learning model, e.g. a neural network model. This approach appears to be appropriate when no accurate physics-based model is feasible (e.g. too complex, too computationally demanding, our understanding is limited i.e. no strong theories). Instead of a physical model of the structure, this approach is data-driven but searches for an optimal fit that respects the physical laws. This approach needs relatively accurate and abundant data but is agnostic with respect to many features of the structure such as boundary conditions and geometry.
C. Hybrid-physics driven approach: using machine learning to improve the safety assessment by the physics-based model by improving the estimation of the input parameter values. This approach appears to be appropriate when the model used can be assumed to be valid both for the assessment of the safety risk as well as for prediction of the responses measured when loads are applied to the structure.
D. Hybrid-data driven approach: the physics-based model is complemented with a machine learning model such as a neural network model that reduces the discrepancy with the response prediction as much as possible. This approach appears to be appropriate when the model used for the assessment of the safety risk cannot be assumed to be sufficiently complete for either the assessment of the safety of the structure or the prediction of response measured when loads are applied, or both.
E. Data-based approach: Fully data driven, no physical consideration are taken into account.

Focus within this ERP is on Hybrid Approach to be incorporated in digital twins (number 2, 3 & 4).

B2. Sensing (depicted as B2 in *Figure 8*)

Acoustics and Fibre Optic Sensing (FOS) technology will be further developed for inspection and monitoring purposes, acting as the eyes and ears of an existing structure. Budget will also be reserved for quick scan techniques.

- Acoustics: In-situ tension measurement and in-situ fatigue state imaging using non-linear ultra-sonics
- Optics: An easy-to-install fibre optic cable for (steel and concrete) bridges that can measure temperature, strain, vibration and acoustics over a large distance, equally distributed along the fibre (distributed sensing).

B3. Validation & Demonstration (depicted as B3 in *Figure 8*)

The data from the 2019 measurement campaign of bridge 705, a concrete bridge located in Amsterdam, marked as bridge 705, is very extensive data set (large number and many different type of sensors) and of high quality. The potential of this data set where measurement is involved hasn't been explored fully. To create an impact in 2020 and kick start future Digital Twin projects the data will be analyzed to further develop the models and sensing technology.

Line C: Existing structures: network - Vehicle load

C1. Vehicle load models

The long term objectives are the development and implementation of a methodology that enables the visualization and prediction of traffic-related information (e.g. traffic loads and intensities) on infrastructure road networks. The owners of the infrastructures can benefit from this information in a manifold of ways, including the (infra)structure-specific assessment and the analysis of the impact of various traffic scenarios (e.g. platooning) on the distribution of heavy vehicles on the network and on the residual life of bridges.

The objectives for 2020 are:

- improvement of the methodology for estimating loads (including the uncertainty of the predictions)
- implementation of the methodology for generating and analyzing scenarios

- analysis of the effectiveness of various sources of information (Bridge WIM as additional WIM station, vehicle counting based on video recognition, information about the origin-destination paths of heavy trucks), based on information already available at TNO or in literature
- software implementation using the CommonSense platform

C2. Steel bridge as Weight in Motion sensor

The overall objective on this topic is to (i) develop knowledge that contributes in supporting clients (like Rijkswaterstaat) in fulfilling their future needs on heavy traffic load information and (ii) develop software that feeds Object and Network Digital Twins with information on traffic loading based on strain sensor measurements on steel bridges.

The specific objectives for 2020 are:

- Gain insight in capabilities of current software for different sensor configurations
- Add capability of weighing multiple (closely spaced) truck axles
- Software (robustness) improvements on most critical aspects
- Formulate initial thoughts about required verification tests

Line D: Design of structures

D1. AI assisted optimization

The main research question of this work package is: *Can algorithmic optimization yield a better design than an engineering approach? If yes, then how much better and how to perform the optimization within reasonable time?* The scope of the question is an entire composite military vehicle subjected to blast and operational loading. The sought for outcome is an entire optimization methodology that can be reused in order to reduce material use, increase safety while significantly reduce the design time, it consists of the following main components:

- Formulation of the problem in terms of design variables/parameters, objective functions, and constraints (with at least one pair of conflicting aspects/requirements).
- Selection of the optimization algorithm that fits the problem.
- Adjustment of the problem formulation to the optimization algorithm.
- Perform sensitivity studies to find design parameters of small importance and in turn to reduce the problem size.
- Perform optimization.
- Evaluate/assess the optimum design.

The optimization algorithm we are looking for (1) can combine multiple models of different fidelity; (2) comes with uncertainty quantification; (3) efficient in terms of the number of function evaluations.

The objectives in 2020 are the same as described above but the scope is limited to (1) a quarter scale composite panel, multiple variants of which were experimentally tested earlier; (2) a single fidelity finite element model. Moreover, a goal is to set up a computational workflow/implementation that can be reused and reused future development and research efforts.

D2 Validation and calibration of material models (Level IV and III) and blueprint bridging level III to II

Within the previous years it was seen that not all failure mechanisms and all physical processes that occur in blast loaded composites are accurately captured with the models that are currently used and available. To provide accurate training material for the AI model, but also to enable a more efficient engineering approach design process, further validation and calibration of the models is needed. One thing that has been missing up till now is an accurate assessment of the material characteristics in the high dynamic loading conditions occurring in blast conditions. This knowledge gap is addressed in 2020.

In the companion project L-AMPV II level II experiments are foreseen. These experiments, as well as the results of the full-scale experiments of Q4 2019 can provide a first reference data set and indication of the bridging of level III and level II. The goal is to develop a blueprint for this bridge in 2020.

D3 Decrease variability in AI supported design by determination of dynamic material parameters

The third WP supports both WP 1 and WP 2. As mentioned, one of the missing links in the project till now is the assessment of the material characteristics for the severe blast conditions. Material properties are normally known at quasi static or low dynamic conditions. No relevant data is found in literature on high dynamic

properties. The current success of the composite blast protector is its high strain rate and through-the-thickness-pressure dependency. Therefore, it is vitally important to determine properties at these specific conditions. Without this knowledge, the number of variables in the design space is much larger (including all material and failure properties) and the uncertainties in the numerical predictions much higher. With less accurate numerical models, the AI techniques do not have the required accuracy of the training material. And as such, the "AI-best design" might not be the actual "best design".

The aim of 2020 is to select the best suitable and available test method to calibrate the FEM material models used to simulate the close-in blast conditions and provide reliable data for the AI-supported design approach.

Results realized

Line A: Digital Twin Technologies

No.	Results planned	Realization
A1	System Requirements for Digital Twin platform	Yes, part in combined report
A2	Prototype implementation Digital Twin platform	Yes, part in combined report
A3	System Design of Digital Twin platform	Yes, part in combined report
A4	Model of structural integrity assessment process of steel bridge, including data flows	Yes, part in combined report
A5	Implementation of demonstrator using Digital Twin platform, including monitoring and asset management data of steel bridge use case	Yes, Bridge 705 was used because of data and model availability, however the developed platform is not bound to a specific bridge. Sematic presentation of the process for IJssel bridge with the real founded values from FEM and probabilistic analysis
A6	Evaluation of data platform based on application in steel bridge DT	Yes, part in combined report
A7	Guidelines and recommendations on the utility and application of various AI assisted modelling approaches	Yes, part in combined report
A8	Prototype implementations of selected AI assisted modelling approaches	Yes and described in a section in the combined report
A9	Demonstration of the utility of selected AI assisted modelling approaches for domain specific use cases	Yes and described in a section in the combined report

Line B: Existing structures: component & structure – Modelling & Sensing

No.	Results planned	Realization
B1	TNO plan use case steel bridge	Yes
B2	TNO report physics based model improvements for steel bridges taking into account the lessons learned from a concrete bridge (bridge 705)	Yes
B3	Test plan for Digital twin modelling approach 'Probabilistic updating' OWT	Yes
B4	Implementation physics based model for advanced prediction of fatigue life of bolts OWT	Yes (B4 & B5 combined in one report)
B5	Test report Digital twin modelling approach 'Probabilistic updating' OWT	Yes (B4 & B5 combined in one report)
B6	Development of EMAT sensors for the purpose of measuring bolt stress in-situ OWT	No Another sensor type was developed instead of using EMAT
B7	Test report of In-situ tension measurement and in-situ fatigue state imaging using non-linear ultra-sonics OWT	Yes
B8	Development of DAS/DVS sensing system for bridges	Yes
B9	Test report evaluating tradeoffs of different types of easy to install fiber optic tested in practical experiments for bridges	No, not a report but a PPT was made
B10	Memo reporting outcome 'quick measurements scan'	Yes
B11	Report ERP DT SI 2020 'physics based model, evaluating the outcome when implementing the physics based model and the improvements suggested for bridges & OWT	Yes
B15/B16	Report "Development of a new methodology for fatigue assessment of complete bolted ring-flange connections for large offshore wind turbine monopiles"	Yes

Line C: Existing structures: network - Vehicle load

No.	Results planned	Realization
C1	Updated version of the Load Map tool (GitLab repository)	Yes
C2	Specification of requirements in terms of type of information source and data accuracy	Yes
C3	Updated Gitlab reporting on Steel bridge as Weight in Motion Sensor	Yes
C4	Updated version of Bridge WIM software suitable for closely spaced axle weighing + prioritized improvements	Yes
C5	Set of requirements for validation testing of Bridge WIM software	Yes
C6	Report about the technology implemented in the Load Map	Yes
C7	Progress presentation(s) that can be shared with potential clients	Yes
C8	Progress presentation(s) Bridge WIM that can be shared with potential clients	Yes

Line D: Design of structures

No.	Results planned	Realization
D1	AI supported best design in limited design space	Yes (80%), (1) the level IV finite element model was not considered as the setup of the computational workflow required more time than expected; (2) further refinement of the mathematical problem formulation is needed, as the current panel integrity evaluation approach has some shortcomings that affect the optimization.
D2	Material models update based on WP 3 results	Yes (60%) the ply failure model was updated. For the interface model the pressure dependency in static conditions was determined and the basic implementation of a user defined interface model was verified
D3	Blueprint bridging scale III to II	Yes
D4	Material characterization data set at high strain rates and under high compressive stresses (release in two batches)	Yes
D5	Report AI techniques for design demonstrated for blast protector case study	Yes (100%), an extensive documentation slide deck is prepared
D5+	AI supported optimization implementation/code repository	Yes (80%), although not explicitly mentioned in the 2020 plan we prepared a well-documented code repository to perform Bayesian optimization where LS-Dyna models are included. Due to licensing troubles the development was mostly done on Azure and using a full, trial license, there was not enough time left to fully adjust the workflow to the HPC and SD-queue (most issues are resolved but some implementation remains).
D6	Report updated material models level IV and III	Yes(60%) the updated relation for the pressure dependency of the shear behaviour at static conditions was determined. The strain rate dependency relations were not done due to late arrival of the dynamic test information (closure of lab due to Corona)
D7	Report material characterisation	Yes (70%) Static tests: analysed and reported, dynamic tests data reported, additional analysis needed.

Realized contribution to new knowledge and technology

Line A: Digital Twin Technologies

The process of integrity assessment of structures is currently a long (two to three years) and resource intensive process (requiring a team of ten people). Digital Twinning is seen as a solution direction that can support solving societal challenges in infrastructures and speed up the process and reduce the required effort. Digital Twins

help in assessment by modelling the structure using a combination of FEM models (using expert knowledge on the bridge) and machine learning models using data from sensors connected. The developed knowledge aimed at getting domain expertise on SI and ICT together and also looking the assessment process itself and how digital means (like sensing, data, digital twin) can facilitate a different 'way of work' in order to solve the challenge of the need for a faster safety assessment of structures.

Line B: Existing structures: component & structure – Modelling & Sensing

This will be described for the three long term objectives set for the use cases Steel Bridge (SB) and Offshore Wind Turbine (OWT).

B1. Dedicated model development

One of the long term objectives when it concerns model development is to create a user friendly platform for the probabilistic calculations and an uniform way to match model data with sensor data. In 2020 an important step was made for the use case 'steel bridge', where the prob-taralli tool was developed on test case 'concrete bridge 705' and test case 'Ijssel bridge'. This will be further enrolled in 2021 using the additional sensor data that has become available for the IJssel bridge and for the living lab 'Moerdijk bridge'.

With the prob-taralli tool it will become possible to:

- Run these calculations at lower cost since we don't need to start from scratch for every new project awarded;
- Get junior's involved in an early stage and have smaller chances in making errors when running the tool.

For the model development within OWT an important step was made in using a new FEM model (akselos)

B2. Sensing

As stated before, sensors are the eyes and ears of the construction and play a very important role to 'sense' global and local behaviour or changes in 'normal' behaviour.

For the ultrasound development important steps have been made to demonstrate the principle and possible limitations to measure stress. The technology will be further developed in 2021 with budget made available from this ERP. The more challenging need to detect voids or cracks in a bolt will be addressed in the 'bolt and beautiful project'.

Focus in the Fibre Optic Sensor development was to further mature the distributed sensing technology. This technology has now reached the stage that it can be used in the Moerdijk bridge, which will be acting as living lab in the upcoming years. It is also aimed for to use the line-like sensor data, generated with distributed FOS, in the prob-taralli tool. This kind of data is new and can be considered as an important milestone if we show that the tool can handle this kind of data sets.

B3. Validation & demonstration

The proof is in eating the pudding. The same holds to explain the idea behind Digital Twin Technologies. Having the demonstrator available for in- and external use, made it possible to show this. We also had to consider this when making the leaflet and the movie and these kind of activities are important to make sure that what we aim for fits with the need of the customer. In our case a bridge owner or the operator of an offshore wind turbine farm.

Line C: Existing structures: network - Vehicle load

For the load map knowledge was acquainted about the statistical description of traffic loads and how this information can be effectively communicated through the use of a web GIS application. The technology position of TNO has improved by an larger degree of knowledge about the traffic loads. In addition the application of GIS technology for a novel use case opens future possibilities. A future collaboration with Rijkswaterstaat and municipalities is envisaged.

For BWiM knowledge on the requirements of BWIM was acquired through literature review and expert consultation. Furthermore the existing algorithms were refined and new algorithms were explored. The technology position has improved since TNO has developed a prototype BWIM system, starting from a proof of concept for one bridge at the beginning of the year. The most likely customer (RWS) has been regularly consulted to inform both parties of the progress and demands from practice.

Line D: Design of structures

The main knowledge contribution a optimization methodology that can be reused in order to reduce material use, increase safety while significantly reduce the design time of military vehicles with new light-weight composite materials. The focus of 202 was on (1) a quarter scale composite panel, multiple variants of which were experimentally tested earlier; and (2) a single fidelity finite element model. To provide accurate training material for the AI model, but also to enable a more efficient engineering approach design process, the models are further validated and calibrated with an accurate assessment of the material characteristics in the high dynamic loading conditions occurring in blast conditions. To understand the characteristics of the composite material better the best suitable and available test method has been selected to calibrate the FEM material models used to simulate the close-in blast conditions and to provide reliable data for the AI-supported design approach.

Realized contribution to the market position

Line A: Digital Twin Technologies

Digital Twinning in the context of Structural Integrity is essentially about making Structural Integrity analyses, in which closer connection is sought with the actual condition and actual load of the object by means of data and sensors. Making these analyses repeatable requires development of 1) assessment methodology and 2) the implementation of this methodology on an IT infrastructure to make the methodology repeatable and scalable. Development of the method includes matters such as AI and FEM, surrogate models, etc., validation of AI (as an alternative to heavy FEM calculation, to make it easier to repeat) and structured data management. To make the analyses reliable, traceable and repeatable, an IT infrastructure is required that is flexible with regard to the number and type of modules that can be linked and that can easily add computing power (by means of cloud technologies and containerisation).

The market potential of TNO is strong because TNO has the unique position to combine deep domain knowledge on Structural Integrity to apply assessments and new techniques (AI, Machine Learning, Bayesian inference) in a meaningful way and make this whole to work on an IT cloud-infrastructure to scale-up analysis in and lower calculation times. For customer assignments also ‘acceptance’ of a other way of safety assessments is needed. These processes take long but also shows a good position for TNO: validate alternatives for the assessment process before the market can pick this up (a true innovation process where TNO explores the risks and undertenancies before companies will pick this up)

Line B: Existing structures: component & structure – Modelling & Sensing

In April 2020 the Hannover Messe fair would haven take place where both BAM and TNO aimed to show the Digital Twin concept by means of a bridge made from plastic parts, a so called demonstrator. Besides the demonstrator, a leaflet was made and a movie so that BAM and TNO could share their vision of DT technologies for existing (infra)structures.

Unfortunately the Hannover Messe (HM) was cancelled due to Covid. Instead an internal tour was organized within TNO where a live demo was presented, similar to the one we had in mind for the HM 2020.

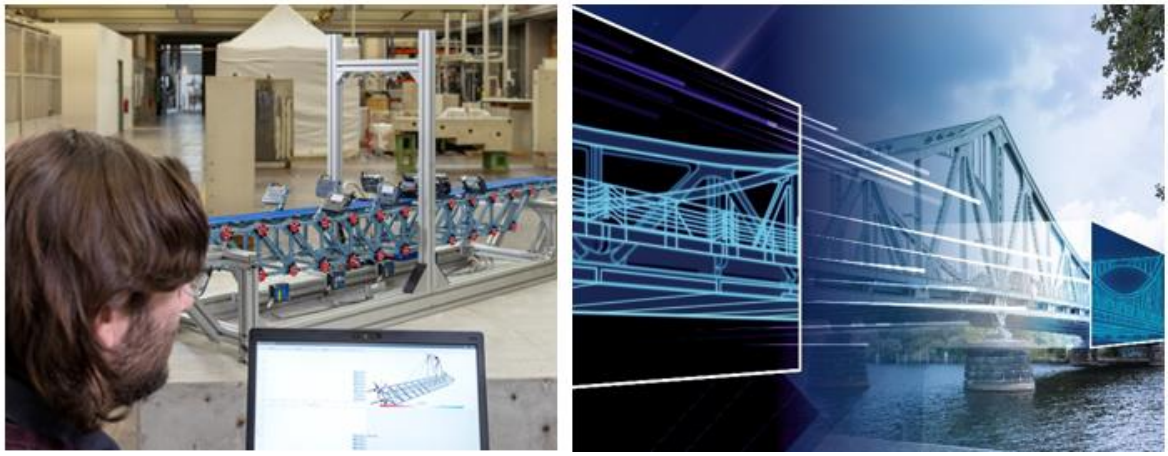

Figure 9: *The demonstrator for the Hannover Messe 2020 & Artist impression ‘Digital Twin’, Copyright: BAM*

Both the demonstrator and the video, intended for the HM 2020, were both well received, and used in and outside TNO. In addition a session was organized by Joep Paulissen to show the potential of this technology and to discuss how we can create impact externally.

Line C: Existing structures: network - Vehicle load

For the load map, TNO positions itself in a unique position on the market. TNO is the only organization that can provide the insight in both detailed information about loads and its spatial distribution. This information is mostly valued by Rijkswaterstaat and municipalities. A workshop with Rijkswaterstaat will be planned to discuss its application and further investigate needs. IP restrictions may be considered for commercial parties that make use of the results. At this moment results are not practically applicable (still in research phase).

For BWiM TNO obtains two possible market positions. Firstly, TNO is developing a BWIM system, which can commercially be exploited if completed. Furthermore, TNO is further establishing its position as the Dutch authority on bridge measurements and its analysis, including BWIM. This is valued by Rijkswaterstaat, provinces and municipalities when acquiring such measurements on the market.

Line D: Design of structures

Over the course of 2020 we increased our theoretical knowledge and hands-on experience with Bayesian optimization for computationally demanding problems. Our results are promising and indicate that algorithmic optimization is feasible and can yield better design than the engineering approach.

The knowledge base on material response of laminate composites under high dynamic loading was significantly enhanced by the combined testing – modelling and the generated data base, which strengthens the TNO market position.

In general

We anticipate that the new capabilities developed in the project will be an important contribution to take a leading position in the international, European team of industries, investigating the developed material as alternative for standard steel solutions, since it most probably will enable a quicker and more optimal design combining all challenges. The resulting faster and improved structure development will create better chances for the realization of improved protection of our military forces. The DT4D and AI developments will support the Original Equipment Manufacturers (OEM) in their design processes. Also, it can create new demands for composite vehicles from the international community of MoD's. Herewith, we build a stronger case for Dutch industry, participating in full scale composite design and manufacturing of composite vehicle structures. Because of the gained leading position of TNO it is the ambition that TNO will be a preferred partner for the industries for the development and/or evaluation of composite (military) vehicles

Publicity

Line A. ***Digital Twin Technologies***

J. Adriaanse et al. TNO 2020 R12196 report 'Design Digital Twin Platform for Structural Integrity'

Line B. ***Existing structures: component & structure – Modelling & Sensing***

- Rózsás, TNO report 2020 10276 'Probabilistic system- and load identification of bridge 705'
- Manai, TNO report 2020 12182 'Model and measurements combination: test case IJssel bridge'
- P. Ochoa, TNO report 2020 11506 Quick scan steel Bridges
- S. van Es, TNO memorandum 'performance test Galecopperbridge of wireless data transmitting of an analog strain gauge'
- R. Pijpers, TNO report 2020 'Development of a new methodology for fatigue assessment of complete bolted ring-flange connections for large offshore wind turbine monopiles'
- Volker, TNO report 2020 'Bolt tension Measurements'
- W. de Jong, pdf document 'TNO DAS datasheet April 2020'
- W. de Jong, TNO memorandum 'DAS blind spot issues' June 2020
- L. Cheng, PPT presentation 'Update Fibre Optic Sensing', June 2020
- R. Jansen; memorandum 'Collaboration topics 2021 BAM and TNO', September 2020

Webinar presentations:

- R. Jansen TNO presentation 'What's next in Fibre Optic Sensing RVO webinar 16 June 2020
- R. Jansen TNO presentation Fibre Optic Sensing NTV bijeenkomst' 24 September 2020 (https://vimeo.com/463012453).

- L. Cheng, 3rd DAS patent ‘Calibration of interferometer response in scattering based distributed fibre sensing system’.

Line D. ***Design of structures***

- D. van Veen, J.Weerheijm. Material characterization through static off-axis compressive testing. Memo 20 EBP/188.
- S.K. Kota, Predicting the failure behavior of off-axis composite laminates subjected to dynamic compression loads. Msc study. TU-Delft/TNO. September 2020.
- J.H.A. Schipperen, ERP DT4D
- J.H.A. Schipperen, ERP DT4D WP3: Numerical analyses off-axis compression tests, TNO report TNO 2020 R11554, 2020
- J.H.A. Schipperen, J. Weerheijm, Blueprint from level III to level II, TNO memorandum TNO-2020-MEM-0100336298
- J.H.A. Schipperen, User-defined contact tiebreak model, TNO memorandum TNO-2020-MEM-0100336297
- J.H.A. Schipperen, Strain rate dependent maximum principal strain failure option for plies in LS-DYNA, TNO-2020-MEM-0100332045

10 ERP ExpoSense

ERP Contacts: Ruben Goudriaan (Project Lead), Stefan Bäumer, Anjoeka Pronk (Lead Scientist), Ardi Dortmans (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

The goal in approximately 10 years is to have developed solutions for personalized promotion of health in the general and work environment based on non-invasive assessment of external and internal exposure profiles. For instance, the development of a 'respiratory health smart watch' which measures air quality exposure, as well as non-invasively measures internal markers of respiratory disease. Continuously, the smart watch provides the user with advice on behavior such as when and where to perform his or her activities for promotion of his or her respiratory health.

The 5-year goal of this ERP is to develop technology for the characterization and interpretation of personal exposure profiles to particulate matter (PM). This technology combines development of novel miniaturized sensors (sense) with sensor-model integration for data interpretation into external and internal personal exposure profiles with respect to health (reason). More specifically, the ERP objectives are:

1. Providing state-of-the-art miniature PM sensors including chemical identification of PM
2. Assessing, interpreting and visualizing real time personal external PM exposure profiles in order to provide relevant advice to reduce the external exposure at the individual and group level
3. Assess and (non-invasively) measure internal markers of PM exposure or a specific chemical component of PM, and relate these to external exposure [1]
4. Building the data technology to enable the future establishment of quantitative relationships between external exposures, internal markers of PM, and forward intermediate health effects, in order to provide relevant advice to reduce health effects [2]

Based on these technologies new personalized or group-based tools can be developed which can give quasi real-time actionable advice in order to reduce PM exposure (act) which can be used to:

- create awareness
- give real time feedback in relation to (occupational) exposure limits
- provide predictions of future exposures (analogous to weather information)
- offer lower exposure alternatives (e.g. cycle routes, playgrounds)
- identify the main sources of exposure in order to guide exposure control measures (e.g. behavior change or use of respirators on the work floor)

These tools, e.g. the respiratory smart watch, will be developed within the relevant VPs in co-development with technology and research partners and in collaboration with end-users. These innovations will take place in several groups of TNO and will strengthen their competitiveness. Next to TNO groups, leading academic groups and institutions will be joined in the ERP: IRAS institute of the University Utrecht, NIOSH (USA), HSE (UK) and several EU projects.

Besides developing technology for personalized promotion of health, TNO will create a network of partners and customers in which knowledge is gathered and brought to the market. Part of the network are the above-mentioned academic networks and EU-projects. Another important network is TI-COAST, where cooperation with companies and universities can be initiated and of course cooperation with companies, who will use TNO technology. The best way of valorization of the TNO technology will be explored and determined case by case.

[1] An initial exploration of the feasibility of using different types of markers for identifying internal exposome is performed under this ERP. This could be succeeded by a new (seed)ERP focused around this topic. The development of noninvasive sensors for internal exposure will not take place within TNO, relevant partners will be connected to the ERP once more insight in 4 has been gained.

[2] The overall integration of these different aspects isseen as very ambitious and pending on the successful development of each individual component. A stepwise approach will be taken, and next development steps will depend on the results of the preceding steps.

Results realized

No.	Results planned	Realization
1.1	Sensor and model requirements	Finalized
1.2	Redesign of micro-cyclone to collect > 95% of all PM in air	Finalized, other dimensions of cyclone
1.3	New inner surface chemistry/morphology of components to reduce accumulation of PM to < 1%	Finalized, metal cyclone instead of plastic one
1.4	Design new air flow scheme to include periodic regeneration of device, having an efficiency of >99%	Finalized, device is regenerated after every measurement, using valves and electronic control
1.5	Increase accuracy of IR based PM counting to at least 50%, having an accuracy in chemical identification of at least 20% (in % of crystalline silica)	Finalized, PM concentration is comparable with commercial sensors, and fraction of crystalline silica is ±15%
1.6	Memo on results of the stakeholder workshop	Finalized
1.7	Memo on progress of occupational exposure modelling in the ERP	Finalized
1.8	Working data infrastructure from sensor-InfluxDB-diamonds-howamIapp	Finalized and demonstrated at Mateboer
1.9	Field test for occupational demonstrator – film or animation showing between 500 – 30000 µg/m^3 PM capabilities with chemical identification of crystalline and amorphous silica	Film production in process, will become available February 2021
2.1	Sensor and model requirements, specifying i.e. update frequency, spatial resolution and type of emissions identified	Partly realized, with respect to the species that need to be detected and corresponding infrared feature.
2.2	Applicability of alternative detectors assessed with the goal of 50% sensitivity gain or 50% cost reduction	In progress and will continue in 2021. PAS assessed as alternative detector: not suitable for PM; alternative hardware feasible, but power budget must be optimized.
2.3	Integration of microcyclone and Virtual Impactor demonstrated to reach 10 µg/m^3 i.s.o. 1000 µg/m^3 particle concentration	Not realized: Virtual Impactor design was expected to be realized in the B2b project with Casella. This has had 6 months delay due to Corona, so integration was not assessed.
2.4	Feasibility of IR-filter based detection demonstrated	Theoretical feasibility of filter-based detection is shown, using dichroic or plasmonic filters. This only requires high power light sources, that will not be wearable.
2.5	Design realized for environmental demonstrator	Initial design is realized, based on modified Arcoptix FTIR having a more integrated footprint, and focusses on environmental PM sources.
2.6	Implementation of improved GPS module towards real time feedback	Implementation in Urban Strategy finalized
3.1	Collaborative project plan detailing the collaboration with non-invasive sensor developer	A collaborative plan with a non-invasive sensor developer has not been achieved, as the validation has been delayed with Aarhus University. A research plan was written instead to describe the steps needed for validation.

	Reports, papers, presentations planned	
1.1	Memo on the description of Demonstrator 1.0	The description of the demonstrator was replaced by an update specification for the sensor
1.2	Report on the adapted PM-CID1.0 sensor	Realized; contains details on the optimization of the mini-cyclone, the demonstrator and the data processing
1.2a	Added: Presentation on the demonstration of PM-CID1.0 for measuring construction dust in outdoor conditions	Realized: demonstration was done in front of Eindhoven HTC25 building.
1.3	Conference presentation of developments and results of PM-CID1.0 sensor	Not realized due to Corona; paper in journal instead
1.4	Paper submitted on IR sensor	Realized and submitted in December
1.5	End user workshop on feedback - TNO news item or publication	Replaced by TNO times publ. of demo movie together with Mateboer – just after film is ready
1.6	Presentation on how context sensors can be used to measure behaviour and applied to control exposure in real time	Abstract submitted, conferences cancelled (covid19), abstract submitted as deliverable.
1.7	Comparison CFD modelling and interpolation techniques for concentration maps – report or draft publication	Outline of paper is ready and submitted as deliverable. Paper will be written and submitted in Q1 2021. To be used for PhD, had no time in Q4 2020. Results were ready.
1.8	Added: Presentation on the final Occupational Demonstrator field test	Realized: Field test was held at Mateboer in Emmeloord
2.1	Memo on the description of Demonstrator 2.0	During 2020, gradually it became clear that the scope for the environmental demonstrator 2.0 in 2021 would change. One of the first activities for 2021 is describing the demonstrator 2.0. Part of this memo is combined with D2.2a with respect to the target species to be detected.
2.2	Memo on the feasibility of alternative detectors (e.g. PAS)	Realized, showing PAS in its current form is not feasible for PM detection
2.2a	Report on the design and progress of the miniaturization activities towards PM-CID2.0 sensor	Realized, including requirements from the environmental demonstrator and possible hardware options.
2.3	Patent application on the filter-based identification solutions	Patent submitted on hollow waveguide sensor.
2.4	Memo on local air pollution modelling (traffic, other sources and validated EU models)	Finalized
2.5	Presentation on the use of TOPAS for source apportionment: both for stationary and personal levels. Mini demonstration of what could be feasible	Merged with D2.4
2.6	Protocol for data collection and validation plan personal exposure profiles by US	Scope of demonstrator 2021 is changed; D2.6 no longer relevant.
2.7	Added: PP describing the GPS module algorithm	Finalized
2.8	Added: Evaluation GPS algorithm	Finalized
3.1	Report validation of PM marker set or plan to create validation data in one of the consortia	The validation has not been completed, but a research plan for validation in Aarhus studies has been completed.

Realized contribution to new knowledge and technology

We have realized the design and construction of a particle sensor that can measure the chemistry of airborne particulate matter in real time (=CID: Chemical IDentifier). This development was based on new designs of a mini-cyclone that concentrates airborne particles 2000-5000 times. The use of the light scattering of particles in the hollow waveguide was used in our advance to calculate particle size and concentration. A new data processing protocol was developed that converts the raw infrared spectrum to quantitative information about the concentration of the individual components in the dust. New insight has been gained in the possibilities of miniaturization of the infrared hardware. New emitter and filter options have been evaluated to enable a smaller sensor concept for the forthcoming demonstrators.

With respect to interpreting and feedback of outdoor PM exposure, we realized the use of high-resolution real-time traffic density data for the whole country instead of just regions improving our air quality estimations. In addition, a new statistical GPS module was implemented in Urban Strategy by which GPS location tracking data can be interpreted in real time and combined with the improved air concentrations of pollutants, resulting in individual air quality exposure profiles. For workplace settings, a proof of principle was conducted in the construction sector in which the PM/CID data were translated into meaningful personal feedback on silica exposure in near real time in an app. In addition, CFD modelling and kriging approaches were used to create indoor concentrations maps based on sensor networks, to be applied in occupational settings.

In terms of linking PM exposure to possible health effects, the activities have led to a finalized list of candidate biomarkers as well as inventory (together with Aarhus) on possible studies were validation of these can be pursued.

The position of TNO in the field of chemical sensors to detect the chemistry of particulate matter has been greatly extended. Not only can we now measure the presence of harmful construction dust, but we have also shown the feasibility of the technology for other components, such as Chromium VI, that will allow the deployment of the technology in a much wider application range. The technology position has been assured by the application of three patents. By adding technology for data communication and interpretation to the developed sensor, we have demonstrated the potential of the application of the sensor into a solution for the occupational setting in which the data is converted into information that can be fed back to the user in real time and allow them to take actions for preventing harmful exposure.

Progress has been made in the area of air quality modelling: connecting high resolution local and regional air quality modelling, linking individual GPS tracks to our air pollution estimations to provide personal exposure profiles, and translation of data into understandable feedback and visualisation thereof in real time through the EXCITE platform. The EXCITE platform can be used for collecting, storing and interpreting high resolution exposure (and health) data in other domains as well. Personal exposures (both occupational and environmental) can now be compared with thresholds in real time, providing a basis for early warning. In addition, personal exposure profiles can be stored and analysed, e.g. for identification of exposure sources or determinants associated with elevated exposure (behaviour, ventilation, weather etc). For this, different modelling approaches are developed, partly also in VP Sustainable Work. In this ERP, we explored indoor dispersion modelling (CFD and Kriging) of occupational exposures in an experimental setting of which Kriging is already embraced in actual field studies in the VP sustainable work.

Exposure to airborne particulate matter (PM) is responsible for about 4% of the disease burden in the Netherlands. Air pollution therefore is an important risk factor, in the same order of magnitude as overweight (5%). The long-term goal (4years +) of this ERP is to develop a personal ‘early warning system’ (e.g. integrated in a wearable/portable device) for PM related exposures consisting of new sensor technology and new interpretation of the data, tuned to each other for best performance. The new challenge in **sensor development** lies in adding chemical identification to the PM sensor, which will allow for better source identification, whereas the innovation in the **data gathering/interpretation** lies in increasing the spatial and temporal resolution: from days to hours and km to m. This combination will warn people in unhealthy situations (e.g. heavily polluted area) and enable corrective actions which in the end should lead to a lower burden of disease. For this an integrated approach is needed for assessing, interpreting and providing feedback on multiple external particulate matter (PM) related exposures and relevant health effects. The ERP Exposense provides potential solutions in the context with the occupational health and public respiratory health domains.

Realized contribution to the market position

The application for the technologies obtained in this ERP are, for example, sensor hardware manufacturers and users and specialists working on (model) data usage and interpretation. Applications for the technologies and systems developed in combination with data valorisation can be found in two main categories:

i. Occupational settings: warning employees and employers if limit values of hazardous substances are reached or providing (groups of) employees with actionable information on when, where and why their exposure levels are elevated. This advice should be given on a personal level or at least on small group level to persons working together. For promoting knowledge on the advantages of the application of sensors for monitoring and management of occupational exposures and for setting up collaborations with different stakeholders (different technology developers and end users), the concept has been concretized as Virtual Industrial Hygiene Assistant (VOHA). A communication campaign is currently being launched (movie: https://www.youtube.com/watch?v=1-S21CpxA_I), and co-development projects will be actively pursued (also in collaboration with VP Sustainable Work). The following projects and activities can be listed so far:

Project / Activity	Type	Project description
Casella sensor development	B2B	Development of a particulate Matter sensor for occupational (construction) dust based on a virtual impactor with electronic detectors
Defence challenge	SMO	Showing the feasibility of the Infrared sensor for toxic analytes
NWA startimpulse	B2B	
5xBeter	B2B	Focus on welding smoke. Knowledge gained on kriging and context sensors is applied within this project.
CBM	B2B	Focus on sawdust. Knowledge gained on kriging and context sensors is applied within this project.
EPHOR	EU	In the EPHOR project, started 2020, the groundwork is laid for evidence-based and cost-effective prevention for improving health at work, by developing a working life exposome toolbox. This is the part of the budget which is closely linked to this ERP project. The total TNO budget is 2.877K. Budget includes EU and SMO contra.
NIOSH / HSE	In-kind	For the occupational application in 2019 / 2020 a joined study together with NIOSH and HSE has been carried out: 3 countries and 3 different settings. The data are available for all parties and is regarded as in-kind contribution of the two cooperating institutes. Data processing and interpretation will continue in 2021.
Market insight construction sector	In-kind	An interest group of 10 Dutch construction companies has been formed to guide the development of the TNO system giving unique market insight. A field study is planned at Mateboer, one of the construction companies.
P4O2: Precision Medicine for more Oxygen	Topsector Health Holland	Development of methodology to monitor indoor air pollution and link this to a disease management system for COPD patients (Monitair solution)

ii. General environment: giving personalized advice on the concentration of pre-defined substances in the air. Based on the advice people will be enabled to make choices on time spent in public spaces. On the modelling research line of the ERP there is a close cooperation with IRAS of the University Utrecht, where per 01.07.2020 a shared post-doc has taken his position (Dr. Kees de Hoogh). Furthermore, an effort will be made to reach out to Fontys Eindhoven for cooperation on population mapping. So far, the following projects and activities can be listed:

Project / Activity	Type	Project description
ILM2.0 Zuid-Oost Brabant	B2B	TNO is partner in a measurement network in Eindhoven and surroundings. TNO is responsible for establishing approximately 50 measurement locations to research regional air quality (375K/yr for 5 years). The Eindhoven network will be used as testbed for new research such as performed in this ERP and future VP demonstrators.
Microplastics in Air	SMO	The usage of the CID for detecting airborne microplastics was explored. Internal TNO budget.
Ammonia in Air	SMO	TNO Brains4Nitrogen project on measuring ammonia in air.
HBM4EU	EU	HBM4EU is coordinating and advancing human biomonitoring in Europe and so provide better evidence of the actual exposure of citizens to chemicals. It additionally provides a robust interpretation of human biomonitoring data and the possible impact of chemical exposure on human health.

For both application areas PM has been chosen as first concrete example, since it related directly to respiratory complaints and has a large burden of disease (4% of all of NL). In addition, several occupational exposures with a high burden of occupational disease are particulate based, e.g. construction dust, wood & agricultural dust, combustion particles, welding fumes.

For the PM sensor itself several additional market segments can be identified:

- Process industry: the application of particle sensors for the control of production processes. This includes e.g. composition monitoring in e.g. food or pharma processes.
- Safety: The presence of airborne dust may lead to hazardous situations, depending on the chemical nature of the dust. Ranging from explosive situations in case of organic dust, to airborne toxic components.

The application areas that are foreseen and evaluated for the sensor technology is shown in the figure. **Error! Reference s ource not found.**The blocks 1 to 4 represent sensor manufacturing markets while 5 to 8 represent end user markets. The parties in green have been contacted during 2020, and some concrete prospects have been established. The parties in orange are identified as an interesting application or partner and will be contacted before mid-2021.

In 2020 several VP activities have been started, which correlate to this picture:

- Smart helmet (VOHA)
- Welding fumes (VOHA)
- Wood dust (VOHA)

There will be follow-up with the relevant parties.

Under this ERP we developed a unique TNO position regarding chemical identification of PM which has been protected in 3 patent applications (2019 – 2020).

Publicity

Publications:

- Núñez, J.; Wang, Y.; Bäumer, S.; Boersma, A., In-line Infrared Chemical Identification of Particulate Matter, *Sensors*, **2020**, *20*, 4193; doi:10.3390/s20154193
- Núñez, J.; Boersma, A., Grand.; Mintova,; Sciacca, B., Ultrathin functional zeolite layer supported on infrared resonant nanoantennas for fast detection of benzene traces, 2020, submitted to ACS Sensors
- Le Feber, M., Jadoenathmisier, T., Goede, H., Kuijpers, E., Pronk, A., 2020. Ethics and Privacy Considerations Before Deploying Sensor Technologies for Exposure Assessment in the Workplace:

Results of a Structured Discussion Amongst Dutch Stakeholders, Annals of Work Exposures and Health, 2020, 1–8 doi: 10.1093/annweh/wxaa093

News items on sensor in the workspace:

- TNO news item: https://www.tno.nl/nl/over-tno/nieuws/2020/3/ethiek-en-privacy-bij-gebruik-van-sensoren-op-de-werkplek/
- https://www.ad.nl/ad-werkt/sensoren-in-werkkleding-moeten-personeel-beschermen-tegen-schadelijke-stoffen~a7dba2b9/
- https://www.engineersonline.nl/nieuws/id32606-ethiek-en-privacy-bij-gebruik-van-sensoren-op-de-werkplek.html
- https://www.privacynieuws.nl/nieuwsoverzicht/databases/166-big-data/21481-ethiek-en-privacy-bij-gebruik-van-sensoren-op-de-werkplek.html
- https://3bplus.nl/sensoren-op-de-werkvloer-vragen-over-ethiek-en-privacy/
- https://www.toxic.nl/nieuws/sensoren-kleding-kunnen-werknemer-tegen-blootstelling-beschermen

Patents:

PLT2019095: "Hollow waveguide for particle identification": filed as EP19207220.5 (filed in 2019)

PLT2019094: IR waveguide with inner coating for gas detection: filed as EP20182025.5

PLT2019125: IR waveguide with outer coating for gas detection: filed as EP20174969.4

11 ERP Future Optical Satellite Communication

ERP Contacts: Cristina Duque (Project Lead), Niek Doelman (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

The main objectives to be accomplished by 2023 are:

- Address the key fundamental and applied research questions in high-speed and secure communication by free-space optical waves and arrive at TRL4 for critical, novel technologies by 2023.
- Connect with academic partners, institutions such as ESA, and industry partners to jointly develop knowledge and technology for future optical satellite communication products. (further detailed in Research Topics).
- Attract external funding for the research program.
- Explore potential cross-overs of the knowledge/technology towards other applications.
- To connect to other National platforms and NWO programs, where applicable.

Research Topics

Given the strong potential of optical carriers waves through free-space, the long-term aim is to arrive at mature technology which fulfils the benefits over RF-waves and/or a fiber network. **The main objective of this ERP is to develop technology for free-space optical (FSO) high-speed and secure communication.** The 'desired technology situation' can be further detailed into four aspects:

a) Performance; much better than with RF-waves, particularly with respect to data throughput and secure communication.
b) Reliability; the performance needs to be guaranteed at any place, any time.
c) Low SWaP/ cost; technology needs to be economically viable, and be compatible with air and space environment.
d) Integration; free-space optical links need to integrated into the overall network (terrestrial fiber-based, RF) and be compatible with standards and beyond 5G for instance.

To meet the desired technology position for TNO and its Eco-system and to fulfil the market potential for Dutch and international industry and service providers, fundamental knowledge and technology (say up to TRL4) needs to be developed. Based on an analysis of a set of use cases for **free-space optical (FSO) high-speed and secure communication,** the following research fields have been defined. These are matching with the existing, and often long-standing TNO's expertise portfolio.

High-speed

- Low loss free-space optical channels, enabling ultra-high data throughput and high key rates
- Mitigation of intensity fluctuations (scintillation) and channel fading
- Modulation and multiplexing for high data throughput
- Modeling of atmospheric turbulence profiles – in particular the statistical behaviour over long periods
- Beam pointing under highly dynamic conditions
- Technologies for multi-point communication
- Orchestration of network traffic to maximize link availability

Secure-specific

- Free-space quantum channels, enabling very high secure key rates
- Optimization of Signal-to-Noise in photon-starved conditions/in day-time operation

Results realized

No.	Results planned	Realization
WP1000	Concept system and Link Budget Optimization for High-Throughput LEO-GRND-LEO links	Partly; work is ongoing
WP1000	Finalization of laboratory tests with multiple channel multiplexer.	Yes
WP1000	Concept for a 3-layer (physical, data and network) optimized scintillation mitigation strategy	Yes
WP1000	Analysis of Cn2-profile statistical model based on meteo-data	Yes, first version of the model. Research is continuing to enhance accuracy
WP1000	Tool to generate Cn2 statistical model for any European OGS-link	Yes, first version
WP1000	Finalization of ground-segment protocol for Advanced Traffic Steering, Switching and Splitting	Yes
WP1000	Concept protocol for traffic orchestration for LEO satellite constellations	No, activity put on hold
WP1000	Concept study of a Low SWaP Photon counting downlink from a Small satellite	Yes
WP2000	Performance analysis of FSO quantum channels for selected QKD protocols	Yes
WP2000	Concept design and analysis of enabling technology for novel, loss-tolerant (beyond PLOB) protocol(s)	Yes
WP2000	Concept design and analysis of a photon-efficient receiver system	Yes
WP3000	Detailed design of a mono-static multi-beam terminal for the aircraft use case	Yes
WP3000	Concept design of a bi-static multi-beam terminal	Yes
WP3000	Development plan for critical technologies in multibeam concepts	Yes
WP4000	Presentations and posters at TNO SATCOMM DAY	No, event has been postponed by 1 year
WP4000	Conference visits, presentations and proceedings papers	Yes
WP4000	Journal publication and patent applications	Yes
WP6000	Contribution to Phase 3 proposal to NWO; Optical Wireless SuperHighways	Yes
WP6000	Research chair progress, PhD deliverables Dissemination Event	Yes
WP7000	Up-to-date and validated roadmap, integration of novel technology candidates, Strategic and tactical review	Yes
WP8000	Strategic and tactical review; progress reports; ERP reports and ERP Plans	Yes
	Deliverables	
WP1000	High Throughput Breadboard report	Yes
WP1000	High Throughput Geo and Leo Feeder Link concept report	Yes (GEO-case), not yet (LEO-case)
WP1230	Report Cn2 profiles	Yes
WP1230	Cn2 script	Yes
WP1240	Demo for5G ground softwarized networks with data splitting	Yes
WP1240	Demo phase 1 5G Leo Networks softwarizations	No
WP1300	Report Concept and roadmap SmallSAT downlink	Yes

WP2200	QKD protocols performance report	Yes
WP2300	Report optical concept and roadmap for QKD protocol with phase locking	Yes
WP2400	Report Concept and roadmap Photon Efficient Receiver	Yes
WP3000	Report Multibeam Design (including baseline selection and trade-off).	Yes
WP3000	Multibeam Development plan	Yes
WP4000	See planned papers, conference presentations, patents (table below)	
WP6000	NWO-TTW proposal (if phase 3 is reached)	Yes
WP6000	PhD Thesis on Control of non-stationary wavefields for Adaptive Optics	Yes
	Reports, papers, presentations planned	
1	Paper to be presented at ICSO 2020	Postponed to April 2021
2	Paper to be presented at Photonics West 2020	Yes
3	2 patents multibeam concept	Under construction
4	1 patent efficient photon receiver	Yes
5	1 patent low-swap downlink concept	Yes
6	Possible patent on Ultra-high throughput GEO concept (currently under investigation)	In preparation
7	Presentations/ posters at TNO SatCommDay	Postponed to 2021

Realized contribution to new knowledge and technology

With reference to the WP structure and numbering the following new knowledge and technology has been acquainted*:*

1000. Ultra-high data throughput

- A refined system concept of a ground communication terminal capable of transmitting data at 10 Terabit/s to a GEO satellite.
- Knowledge on how to minimize the impact of channel scintillations by an optimized combination of spatial diversity, coding, error correction and adaptive optics.
- Knowledge on various concepts to combine high power wavelength multiplexed beams (~50) into a single (> 1 kW) transmitted beam.
- Further advancements in technology and experimental set-up to verify the performance of a grating for high power beam combining.
- Knowledge on how to convert meteo-data to estimate a Cn2-profile for any earth-to-space link.
- Knowledge and simulation tool and how to split data between multiple ground stations for a feeder link to a GEO satellite.
- Knowledge and concept of a laser source for a very low SWaP optical communication terminal at a Small satellite

2000. Ultra-secure communication

- Knowledge on the potential and the limitations on the achievable secure key-rate and quantum bit error for satellite-based QKD protocols; in particular BB84, COW, CV-QKD, MDI
- System concept for a high secure key rate optical channel for BB84 from a LEO-satellite.
- Knowledge on how to achieve a very high rejection of background light in day-time QKD applications.
- Knowledge on phase-locking concepts to enable TwinField QKD.

3000. Multi-point communication

- System concept of a GEO communication terminal capable of receiving and transmitting data from and to multiple users;– design based on a mono-static principle.
- System concept of a GEO communication terminal capable of receiving and transmitting data from and to multiple users; specifically for multiple aircraft – design based on a bi-static principle.
- Consolidated design for the use case of multiple aircraft.

6000. University research

- Knowledge of optimal filter approaches to handle angular anisoplanatism in Adaptive Optics.
- Knowledge and concepts for wavefront phase prediction in direct exoplanet imaging
  - Performance analysis or the VLT-AOF-Sphere instrument

    - Analysis of the Periodic brightening of Kepler light curves
- Knowledge and a system concept of direct dark-zone contrast optimization by an adaptive coronagraph for exoplanet imaging.
    - Analysis for a large variety of dark zones
    - Method to estimate non-common-path aberrations
    - Machine learning approach to improve the tracking speed of the contrast controller.

This project has a significant effect on strengthening the TNO technology position since it builds the key knowledge and technology fundament for future projects (technology development and product realization) with Dutch and international industries in optical communication. In particular, it helps in creating a sustainable strong technology position for high-speed and secure communication by free-space optical waves.

Realized contribution to the market position

This ERP project mainly addresses the lower TRL regions of technology development (say TRL 1-4). Successful completion within the ERP means that the technology has moved closer towards commercial realization and product development. With the 2020 project results the market position has been improved, specifically with respect to the target fields of high-speed communication and secure communication. Potential products from this ERP are: feeder link ground terminal, high power beam combiner, low scintillation transmitter, quantum channel (Tx, Rx) for QKD, multi-point communication space terminal, protocol for feeder link network, wide FoV space telescope, background filter, and more.

Commercialization or joint development with industrial partners will be followed through once the required TRL has been reached. Most potential industrial partners are already linked to the Laser SatComm program. In the upcoming years (Dutch) industry will be involved in the development of prototypes of the foreseen products.

Specifically in 2020: a TKi project is running on high power beam combining with Hittech, a TKi project is running on a QKD system with ABN, a TKi project is running on GEO-satellite based QKD system with Eutelsat, an ESA project is running on a photon-efficient receiver for a deep-space communication system ,..

IP protection is performed along the lines of the Optical Satellite Communication IP strategy. Where feasible a patent is applied for. Or if more suited: a trademark, design or copyright. Any research and concept design documented is put in an I-depot.

Publicity

Publications (reports, books, papers, presentations, websites etc.):

- Silvestri et al., "*Beam Multiplexing for Satellite Communication Optical Feeder Links*", SPIE Photonics West conference, Proceedings Volume 11272, Free-Space Laser Communications XXXII; 1127213 (2020) https://doi.org/10.1117/12.2543035
- Radakrishnan, Keller and Doelman, "*Contrast control of adaptive optics for direct exoplanet imaging*", submitted to SPIE Journal of Astronomical Telescopes, Instruments, and Systems.
- Radakrishnan, Keller and Doelman, "*Measuring non-common path aberrations in adaptive coronagraphic systems*", submitted to Astronomy& Astrophysics.
- vanKooten, Doelman and Kenworthy, "*Robustness of prediction for extreme adaptive optics systems under various observing conditions - An analysis using VLT/SPHERE adaptive optics data*", Astronomy & Astrophysics, Volume 636 (April 2020) A&A, 636 (2020).
- Doelman, "*The minimum of the time-delay wavefront error in Adaptive Optics*", Monthly Notices of the Royal Astronomical Society, Volume 491, Issue 4, February 2020, Pages 4719–4723.
- vanKooten, Kenworthy and Doelman, "*Periodic brightening of Kepler light curves: investigating the possibility of forward scattering due to dust clouds*", Monthly Notices of the Royal Astronomical Society, Volume 499, Issue 2, December 2020, Pages 2817–2825.
- vanKooten, "*Predicting the Future – Predictive Control for Astronomical Adaptive Optics*", PhD Thesis, Leiden University, 2020.

Patent applications:

- AO enhanced Photonic Lantern; TNO ref: 2019114, being assesses by EPO.
- Ultra-low SWaP high capacity links; TNO ref. 2019115, being assessed by EPO.

On "Bulk Multiplexer concept", in preparation for submission.

12 ERP Wise Policy Making

ERP Contacts: Josephine Sassen (Project Lead), Leon Kester (Lead Scientist), Hendrik-Jan van Veen (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

Our ambition for 2022 is to deliver a prototype (TRL 5) of a 'Wise Policy Suite'. With this Wise Policy Suite, we will be able 1) to assist policy makers in quantifying the impacts of different policy options on wellbeing, and 2) to have fruitful dialogues about the policy options and deliberate on the impacts with each other, citizens and other stakeholders. The Wise Policy Suite' consists of instruments and methods that are tested and validated in practice, and are geared towards practical use by policy makers. This will enable them to develop and choose policy options that maximally promote wellbeing, based on scientific insights and demonstrably legitimized by society. There are 3 main lines of research:

1. *WISE Cube (formerly 'EIWA'):* The WISE Cube is an ex-ante evaluation instrument to support policymakers in prioritizing and steering policies towards societal wellbeing. It is an interactive tool that gives a visual forecast of the effect of an intended policy measure on the sustainable wellbeing for the relevant parties that this policy concerns. The tool helps to assess the impact of policy options on wellbeing by quantifying the impacts using valid wellbeing models and data. The Wise Cube can be used for policy options in any domain, filling it each time it is used with the relevant data and context-specific relations. We will further develop our current prototype from TRL 3 to TRL 5.
2. *WISE Tank:* The WISE Tank is complementary to the Cube and contains a set of methods that help policymakers and stakeholders to conduct a well-structured, unbiased, 'wise' dialogue about policy options. Supported by an advanced formal dialogue representation tool, the participants are guided to reason in the discussion from values that they consider important, not only for themselves or their "sector" but also for later and for common well-being. The dialogue is used to map the most relevant values and knowledge for the policy options. The arguments for and against options, and the underlying facts, knowledge and values, are registered so the decision of the WISE Tank is transparent, explainable and can be stored for later reference. In this way, the WISE Tank complements the outcomes of the WISE Cube by supporting policy discussions on the outcome of the WISE Cube.

Policy Practice: This line of research is about demonstrating, evaluating and tuning the results from the WISE Cube and WISE Tank based on their concrete use in actual policy practices. It encompasses an extensive case study on how wellbeing-oriented policy making is approached and implemented in actual real-life cases such as in Scotland and New Zealand, the current frontrunners. Based on these empirical insights we are shaping and conducting a set of iterative experiments that test the WISE Cube and WISE Tank in practice. This effort is geared towards making the tools in the Wise Policy Suite work for policy processes. The above instruments will be tuned to actual policy practice in specific domain contexts, with as a first use case: decision making on the Future Sustainable Urban Mobility System. Simultaneously, we are experiencing much interest and active participation from policymakers in the field of Security and Safety (i.e., NCTV) which might make it possible to also address a case study in that field.

Results realized

WP1: Wise Cube (formerly: EIWA)

No.	Results planned	Realization
1.1	Prototype (MVP) EIWA data collection component	No Still important and will be taken up but we rearranged the schedule because new insights led us to realize that we *first* needed to build the case study (future sustainable mobility) and advanced DCM & MARVEL before it was useful to look at the data component. We will put full focus on this deliverable in 2021 as it is the biggest next step in further developing the WISE Cube
1.2	Prototype (MVP) EIWA quantitative model component	Yes

1.3	Prototype (MVP) EIWA interactive dashboard component	Yes
1.4	Interim rapport concerning the prototyping approach and results	Yes
	and on methodologies to compensate for cognitive biases focusing on the EIWA components	Yes: This deliverable is partly achieved and partly the need for this deliverable has been diminished. We have published an article on biases but we did not relate it to the prototyping approach as this did not seem of much added value in retrospect

WP3: Wise Tank

No.	**Results planned**	**Realization**
2.1	Report on dialogue representation theory and argumentation mining and its potential to enhance existing tools to improve policy dialogues	yes
2.2	Work document on the potential of Marvel and first draft of description of role of Dialogue support in Wise Tank	yes
2.3	Knowledge on the theory of argumentation mining with special attention for its potential role in widening the scope of a policy dialogue.	yes
2.4	Report with a critical analysis of the wisdom literature, conceptions, and models with special attention for 'collective wisdom' in policy making	yes
2.5	Report on critical biases that prevent adequate decision making in sustainability policymaking	yes
Extra	Conference presentations and (concept) publications on how to foster (collective) wisdom in policy making, and on the origin and mitigation of cognitive biases in decision making Extra TNO report, intended for practical use, including a concise presentation of (the background of) the Neuro-Evolutionary Bias Framework.	yes

WP3: Policy Practice

No.	**Results planned**	**Realization**
3.1	Report on the State of the Art in assessment mechanisms and decision making models currently used in the domain of Future Sustainable Mobility	Yes. These reports have been combined into one deliverable (3.1 and 3.2)
3.2	Report on survey among policy makers regarding the relevant parameters to be used in impact assessments, issues and dilemma's concerning current usage of these parameters in impact assessments, and the added value of EIWA and Wise Tank tooling	
3.3	A clear use case description for the use case future sustainable mobility, including a description of EIWA indicators and the Wise Tank process	yes
3.4	Stakeholder assessments of the added value of EIWA and Wise Tank methods for the future sustainability use case	yes

Realized contribution to new knowledge and technology

On the basis of the state of the art in 'beyond GDP', we have seen that there are various indicators available to evaluate wellbeing in retrospect (ex-post). There are, however, currently only few and very limited instruments to assess wellbeing effects of policies prospectively (ex-ante). Ex-ante policy evaluations such as social cost-benefit analysis, multi-actor multi-criteria analysis, and social impact assessment, include measurements that touch on wellbeing. However, these do not include the conceptual refinement and scope of measurement possibilities as developed in the literature on positive psychology and 'post-GDP' indicators. This means that ex-ante policy assessment could benefit from having more integrated and comprehensive measures of wellbeing at its disposal.

Among the current (persistent) challenges of ex-ante evaluation are the scope of the analysis, the determination, choice, and weighting of different indicators, and the costs of actually executing such analyses as well as gathering the necessary data; thus there are many missing and incomplete pieces to the puzzle. This ERP is

finding a way to bring the ‘pieces of the puzzle’ (we call them building blocks) together, all of which have their roots in various scientific domains/disciplines. TNO has the advantage that it has all of these disciplines ‘in house’ and is furthermore recognised for its unique ability to bring disciplines together, which gives us ‘right to play’. Perhaps this is why we are the first in the world to do so.

Most of the building blocks themselves need refinement or improvement too. While we are ensuring a good fit for all of the building blocks, we are surpassing the existing state of the art by innovating on two of the building blocks: Discrete Choice Modelling and Neuro Evolutionary Biases.

Discrete Choice Modelling

In the academic literature there are examples of how discrete choice models can be used to predict transport mode choice, but these approaches are often not fitted to rich data sets, do not take regret minimalization and los aversion (bias) into account and are not related to wellbeing effects. We developed an integrated data set to predict mode choice for the Netherlands and fitted a Discrete Choice Model based on regret minimalization to capture the loss aversion bias.

Neuro evolutionary Biases Framework

A large body of literature shows how cognitive biases may lead to suboptimal or unwise decisions in a broad range of situations, including policy making. However, these studies do not sufficiently explain why biases are so pervasive, specific, and persistent, even under conditions without complexity, uncertainty, or time pressure. In this ERP, we have developed a Neuro-evolutionary Bias Framework that has been published and has already been accepted to be taken up in the prestigious Encyclopedia of Behavioral Neuroscience. This Bias Framework provides insight into the neuro-evolutionary origin and underlying working mechanisms of cognitive biases. This gives us a firm handhold on how to handle and/or mitigate biases and how to use this knowledge to promote better and more wise decision making, that is: policy making supported by methods, tools and interventions aimed at long-term wellbeing.

Realized contribution to the market position

This is an important question to answer. We have taken up this question with our CEO Paul de Krom and other strategic managers at TNO among whom Erik Drop, Frans van Gemerden and Rogier van Keulen. Launching a key enabling methodology (KEM) based on principles of social innovation (meaning the innovation results in changes in how people think, feel, act and/or reflect) pertains directly to TNO’s strategic goals. Though a *direct* effect on turnover or an increase in customers is also likely in the longer run, the most important effects will be in our market position as

- a trusted partner of government
- a trailblazer in addressing wicked societal problems (by means of transdisciplinary science)

This research contributes to the 2 roadmaps of T&T and the National Security roadmap of DSS. In both roadmaps we foresee that Wise policy Making will be taken up in Vraaggestuurde Programma’s and/or SMO. Furthermore we are exploring the relevance of this ERP for the roadmaps of SA&P and Healthy Living. Finally, there is shown interest from the Nationale Coordinator Terrorismebestrijding en Veiligheid (NCTV), the municipality of Rotterdam and the ministry of I&W.

Publicity

Publications

- Korteling, J.E., Sassen-van Meer & Toet, A. (2020). *Neuro-evolutionary framework for cognitive biases*. Rapport TNO 2020R10611. Soesterberg: TNO Defence, Safety & Security
- Korteling, J.E. (2020). *Neuro-evolutionary bias framework*. Draft Memorandum Soesterberg: TNO Defence, Safety & Security
- Miedema, H.M.E. (2020) *Dialogue Representation: Static States of Description and Prescription, and their Transitions* (submitted for publication)
- Korteling, J.E., (2020). *Critical biases for methods and tools for Dialogue Support*. Report paper TNO-DSS.
- Korteling, J.E., Gerritsma,J. & Toet, A (2020). Retention and Transfer of Cognitive Bias Mitigation Interventions: A Systematic Literature Study. Draft publication to be submitted to: *Frontiers in Psychology*
- Korteling, J.E., Sassen-Van Meer, J. Paradies, G. (2020). *Critical biases in policy making for sustainability*. Draft Report. Soesterberg: TNO Defence, Safety & Security
- Korteling, J.E. & Toet, A. (2020). Cognitive biases. *Encyclopedia of Behavioral Neuroscience 2nd edition*. Amsterdam-Edinburgh: Elsevier Science.

- "*Sustainable AI Safety?",* Nadisha-Marie Aliman, Leon Kester, Peter Werkhoven and Soenke Ziesche, Delphi Journal (Interdisciplinary Review of Emerging Technologies), 2020
- Key note on: "*XR for Augmented Utilitarianism*", Nadisha-Marie Aliman, Leon Kester and Peter Werkhoven, IEEE International Conference on Artificial Intelligence and Virtual Reality (AIVR December 2019)
- "*Extending Socio-technological Reality for Ethics in Artificial Intelligent Systems*", Nadisha-Marie Aliman and Leon Kester, IEEE International Conference on Artificial Intelligence and Virtual Reality (AIVR December 2019)
- Steen, M., Bouman, M.J., Sassen-Van Meer, J.P., Van Dongen K., & Vonk, T. (2020). 'Organizing Transdisciplinary Innovation Projects', conference paper presented at ISPIM 2020.
- Master thesis, Wicorel van der Pol, 'The accumulated regret of trip chaining': Here an alternative Discrete Choice model was developed and fitted to the database based on regret minimalization to capture the loss aversion bias

13 ERP STAR-PV

ERP Contacts: Ando Kuypers (Project Lead), Mirjam Theelen (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

To improve reliability and sustainability, reduce cost and reduce environmental impact, the objective of the project is to achieve more predictable and longer lifetimes of embedded optoelectronic devices in multi-stress environments, through a model-based understanding of degradation mechanisms. To achieve this, post mortem analysis of devices failed in the field is used to guide accelerated lifetime testing in the lab, in combined-stress tests.

Reliability and stability of opto-electrical devices in general is very broad and not all topics can be covered. In order to obtain optimal synergy from the collaboration between Holst Centre, STA (Solliance) and SE (Petten) several topics were selected which are generic between the selected technology lines:

- Potentially (semi-)flexible PV: CIGS and x-Si (higher TRL), perovskites and integration in tandems (lower TRL);
- Flexible and stretchable electronics.

During 2020, the objective has been narrowed down to more specifically develop a basic understanding of relevant degradation mechanisms at (1) the interfaces of and within the active and functional PV layer materials (CIGS, PSC, x-Si), of (2) the flexible / ductile electrical interconnects (PV, device applications for medical and healthcare) and of (3) the encapsulation material after exposure to selected accelerated stress conditions.

Results realized

No.	Results planned	Realization
R1	Partial shadowing degradation mechanisms determined in full module by coring	Yes
R2	PID degradation mechanism determined in full module by coring	Yes
R3	General degradation mechanisms for partial shadowing proposed	Yes
R4	Definition and submission of parallel PhD project on PSC or PSC-tandem stability issues, and actively involve PhD TUD on MeO_x passivation of x-Si in the reliability testing of this layer	Yes (TUD PhD PSC financed, PhD MeOx actively involved 2020)
R5	Perovskites as well as c-Si devices degraded under combined stress loads of humidity, elevated temperatures and illumination	Yes
R6	Introduction of MPP tracking for 30+ devices under continuous analysis	Yes
R7	Testing of CIGS devices under various atmospheric gases (N_2, O_2, CO_2 and H_2O vapor)	Yes (setup realized, tests started)
R8	Reliability testing of Back Contact x-Si laminates using novel encapsulants designed for disassembly	Delayed (supply of encapsulant rescheduled for 2021)
R9	Introduction of mechanical vibration testing methods for PV modules simulating practical stress conditions in floating PV, Infrastructure Integrated PV	Yes (started in Q4 in collaboration with TNO BIM)
	Reports, papers, and presentations planned	
R1	At least 6 conference presentations (indicative: STA 3, SE 2, Holst 1)	Yes (6 presentations, 6 posters)
R2	At least 8 submitted scientific manuscripts (indicative: STA 4, SE 2, Holst 1)	Yes (6 published,1 submitted, 3 master theses)
R3	At least 3-4 submitted patents (indicative: Holst 2, STA 1, SE 1) *See also under 6*	Partly (earlier 2 to PCT phase, 2 not filed but confidential knowhow)
R4	Progress report listing identified failure modes by post-mortem analysis of field exposed PV modules (mechanical isolation of defects and lab analysis)	Yes
R5	Report on effectiveness meander structures in stretchable interconnections	Yes

R6	Progress report on mechanical stress induced degradation in stretchable printed interconnection lines	Partly (initial internal report created)
R7	Internal report describing reliable and proven degradation test method for testing modules with encapsulants designed for easier module dismantling under water or temperature treatment.	Delayed (supply of encapsulant rescheduled for 2021)
R8	Internal report on application specific degradation testing of customized x-Si modules with innovative module materials. (selected PV modules for floating solar, BIPV, automotive, I2PV)	Partly (initial internal report created)
R9	Progress report listing identified failure modes and mechanisms in x-Si modules using MeOx and poly-Si passivation layers	Yes
R10	External publication of TNO position paper on circularity/sustainability integrated PV (BIPV)	Yes (internal report finished, external will be aligned with TNO position paper Solar 2021)

Realized contribution to new knowledge and technology

- Post mortem analysis of field degraded PV modules: A novel reproducible method to extract small, still functional samples from larger PV devices by hollow diamond drilling (“coring”) as well as a novel method to remove the encapsulating glass and polymers without damaging the functional device layers. As the resulting samples are still a complete device, they can be optically and electrically analysed in detail
- As the above mentioned disassembly was performed on samples from multiple suppliers, it was learnt that considerable variations occurred in ease/difficulty of disassembly of specific encapsulants. Thus combined information on device reliability as a function of encapsulation method, as well as device recyclability as a function of encapsulant properties can be revealed.
- Methods and equipment for novel multiple stress tests, simulating real and representative combinations of stress in
- integrated PV applications: real time monitoring of device properties under combined humidity/temperature/irradiation/electrical load conditions, combination with specific mechanical stresses (prolonged stress, vibration, excessive load, impact)
- A more fundamental understanding of thin film (CIGS) PV degradation under partial shadowing conditions as encountered in integrated PV applications (buildings, cars, roads, infrastructure). Potential methods for mitigation of such degradation have been identified or proposed, and will be explored for improved stability against partial shadowing: intrinsically, or by electronic solutions.
- Material analysis based fundamental understanding of migration effects (e.g. Na-migration in CIGS) taking place under combined stress conditions with electrical load (reverse bias, PID); also methods for mitigation have been identified and tested (e.g. diffusion barriers, controlled Na-supply, voltage induced reversibility)
- Understanding (modeling and validation) of localized deformation of printed conductive lines, resulting in design rules for stretchable interconnects, applications in wearable vital sign patches and smart clothing
- Optimised designs for printed flexible and stretchable interconnects in opto-electronic devices and flexible photovoltaics
- Degradation studies of silicon PV electrical interconnections upon exposure to Damp Heat and PID stress conditions are performed under influence of different encapsulant materials (EVA, PO and specifically modified encapsulants); basic insights have been obtained for EVA (release of interconnect degrading chemicals under water ingress). This knowledge also provided insight in similar degradation observed in field degraded thin film CIGS.
- Summary of LCA literature and (BI)PV sustainability legislation (under development) as basis for TNO wide joint position paper (generation of new knowledge).

In most of these cases, the knowledge of the identified degradation mechanisms can be used to provide mitigating solutions for PV process and device development at TNO. Also, on the longer term, critical design parameters for specific integrated PV applications can be identified and made quantitative, and translated in to improved integration methods. Thus expanding the potential of PV as a ubiquitous source of durable energy.

Realized contribution to the market position

The ERP STAR greatly improves the market position of TNO as it focuses on novel reliability issues which arise now that the growing scale of photovoltaics dictates multiple use of available surface. Parties higher up the value chain (investors, owners, users, insurance companies, etc) require improved reliability and predictable lifetime of PV which is no longer operated stand-alone, but integrated in specific environments in which the devices are

exposed to combined stress factors. Through the post mortem analysis approach we are now able to perform in depth lab analysis on samples taken from field exposed devices which show failure or degradation, and to develop representative accelerated lifetime tests in the lab. This we can use to evaluate and test proposed device improvements which can mitigate the degradation problems.

Opto-electronic devices are becoming cheap commodities, they are increasingly used in (integrated) applications where they are exposed to multiple stress factors. Understanding, monitoring and improving the reliability of such devices will increase the lifetime and the sustainability of the products. The gained insight of these combined factors will strengthen TNOs knowledge position in the field of reliability and sustainability.

With the thus developed methodology and device specific insights, we are able to address the whole value chain from producer to end user/investor/insurance company. In this ERP, and its parallel projects which are now developed, we extend our network with partners along this value chain, and with universities. Participation in such networks on national and EU level has been made part of the project activities, and specifically with respect to sustainability, impact and visibility will be increased by a position paper in 2021.

Results are protected by patents on device improvements and confidential know how on methodology. A spin off is that the methodology to reproducibly disassemble test samples provides ideas for recycling strategies.

Publicity

Conference presentations:

- EuroCORR, Degradation of CIGS solar cells due to the migration of alkali-elements, Mirjam Theelen, Vincent Hans, Nicolas Barreau, Henk Steijvers, Zeger Vroon, Miro Zeman, September 10th 2020 (oral, virtual conference)
- EUPVSEC, A systematic approach to assess the environmental impact of new technologies: A case study for CIGS PV, Mitchell van der Hulst, Mark Huijbregts, Niels van Loon, Lucinda Kootstra, Joseph Bergesen, Mirjam Theelen, Mara Hauck, September 10th 2020 (oral, virtual conference)
- R. Aninat, K. Bakker, L. Jouard, M. Campillay, G. Gomez, and M. Theelen. “Shunting defects induced by shading on a Cd-free commercial CIGS module”. In: eMRS. Oral 2020 (virtual conference).
- K. Bakker, H. Nilsson Ahman, N. Barreau, K. Aantjes, T. Burgers, A. Weeber, and M. Theelen. “Propagation mechanism of wormlike defects in CIGS solar cells”. In EuroCORR. oral 2020 (virtual conference)
- K. Bakker, A. Rasia, S. Assen, B. Ben Said Aflouat, A. Weeber, and M. Theelen. “How the absorber influences the formation of reverse bias induced defects in CIGS solar cells”. In: EUPVSEC. oral. 2020 (virtual conference)
- P. Yilmaz, R. Aninat, G. Ott Cruz, T. Weber, J. Schmitz, and M. Theelen. “Post-Mortem Analysis of CIGS Solar Modules failed due to Potential Induced Degradation (PID)”. In: eMRS. oral. 2020. (virtual conference).

Conference posters:

- K. Bakker, A. Rasia, S. Assen, B. Ben Said Aflouat, A. Weeber, and M. Theelen. “How the absorber influences the formation of reverse bias induced defects in CIGS solar cells”. In: eMRS. poster. 2020.
- A. Kingma, D. Roosen, S. Kulkarni, M. van den Nieuwenhof, K. Bakker, P. Toonssen, and M. Theelen. “Reliability studies of rigid and flexible Cu(In,Ga)Se2 devices with thermography and luminescence techniques”. In: NREL PVRW. poster. 2020.
- M. Theelen, R. Hendrikx, N. Barreau, H. Steijvers, and A. Boottger. “The effect of damp heat illumination exposure on CIGS solar cells: a combined XRD and electrical characterization study”. In: eMRS. poster. 2020.
- P. Yilmaz, R. Aninat, G. Ott Cruz, T. Weber, J. Schmitz, and M. Theelen. “Defect Investigation by “Coring” for CIGS Solar Modules”. In: EUPVSEC. poster. 2020.
- P.M. Sommeling, J. Liu, J.M. Kroon. “Post mortem analysis of bifacial PV modules based on N-type crystalline-Si cells using three different types of encapsulants”. In: EUPVSEC. poster September 7th 2020.
- P. van Dongen, C. Kjellander. MYSA, A shirt to breathe more consciously through vibrotactile feedback “MYSA, A shirt to breathe more consciously through vibrotactile feedback” EuroHaptics 2020, Leiden, Netherlands, September 6th – 9th, 2020.

Scientific publications:

- G. de Amorim Soares, J. Carolus, M. Daenen, A. Masolin, T. Birrenbach, A. Gerber, A. Wrigley, J. Henzel, D. Roosen, M. Meuris, M. Theelen, Round-robin of Damp Heat Tests Using CIGS Solar Cells, accepted in Solar Energy (2020) https://doi.org/10.1016/j.solener.2020.11.048

- M. Theelen, V. Ntinas, H. Steijvers, H. 't Mannetje, Z. Vroon, The influence of substrate glasses on the damp heat degradation of ZnO:Al films, Thin Solid Films 715 (2020) 138429). https://doi.org/10.1016/j.tsf.2020.138429
- K. Bakker, A. Rasia, S. Assen, B. Ben Said Aflouat, A. Weeber and M. Theelen, How the absorber thickness influences the formation of reverse bias induced defects in CIGS solar cells, EPJ Photovoltaics 11, 9 (2020) https://doi.org/10.1051/epjpv/2020006
- M. van der Hulst, M. Hauck, L. Kootstra, M. Theelen, N. van Loon, J. Bergesen, M. Huijbregts, A stepwise approach to assess the environmental impact of new technologies, Journal of Industrial Ecology 24 (6) (2020) 1234-1249 https://doi.org/10.1111/jiec.13027
- K. Bakker, H. Nilsson Åhman, T. Burgers, N. Barreau, A. Weeber and M. Theelen, Propagation mechanism of reverse bias induced defects in Cu(In,Ga)Se2 solar cells, Solar Energy Materials and Solar Cells 205 (2020) 110249
- Yury Smirnov, Laura Schmengler, Riemer Kuik, Pierre-Alexis Repecaud, Mehrdad Najafi, Dong Zhang, Mirjam Theelen, Erkan Aydin, Sjoerd Veenstra, Stefaan De Wolf, Monica Morales-Masis, Scalable Pulsed Laser Deposition of Transparent Rear Electrode for Perovskite Solar Cells, accepted in Advanced Materials Technologies (2020)
- C. Hagedoorn, M. Götz, N. Neugebohrn, A. Weeber, M. Theelen, Damp Heat-Induced Degradation Mechanisms occuring in colored oxide/metal/oxide films for Thin Film Solar Cells, submitted to Thin Solid Films (2020)

University master theses:
- Brian Dirven, Aging of semi-transparent mixed-halide perovskite solar cells: the effect of illumination and orientation on stability. Master thesis TU/e, 2020
- M. Gonzalo Ott Cruz., Post-Mortem Analysis of CIGS Solar Cells with Coring Activities, Master thesis Universidad Tecnica Federico Santa Maria (2020)
- Vidya Chandrasekhar Krishnan, Mechanisms of Degradation in Perovskite Solar Cells and Modules: A Review, , Master thesis TU Delft, 2020

TNO reports:
- P. Bouten: Mechanical test equipment for stretchable conductive materials, TN-19-SiF-HPE-036, TNO Holst, July 2020
- P. Bouten: Mechanical tests on printed conductive lines; Resistance increase of meanders on stretchable substrates; TN-20-SiF-HPE-002; TNO Holst, July 2020
- M. Hauck, R. Nijman, S. van Leeuwen, L. de Simon: Sustainability Assessment of PV, with attention to the built environment, TNO CAS, Dec 2020

Patent descriptions, premier depots

Two patents that were filed around the start of the project have reached PCT phase (PLT2019022 Metal wrap through for thin film multi-junction solar cells, and PLT2019041 Method to manufacture self-protective flexible PV semi-fabricate), while another patent idea (TMA to reduce side ingress of moisture) still waits for a demonstration example of the principle.

The envisaged patenting of the sample disassembly method, also as a possible route towards recycling with higher rest value, has been decided to rather be protected as confidential know how.

14 ERP Large-Area Ultrasound

ERP Contacts: Jan-Laurens vd Steen / Gerwin Gelinck (Project Lead), Paul van Neer, Laurens Peters (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

Ultrasound for medical imaging and diagnostics has evolved into some of the most valuable medical diagnostic modalities. The diagnostic imaging capabilities of ultrasound have spread across many clinical applications, from obstetrics and gynecology, orthopedics and cardiology, to emergency medicine, breast cancer detection and more. The portability of ultrasound systems, speed, absence of ionizing radiation and cost-effectiveness are some of the key attributes that have given this technology an edge over other imaging modalities. An important new development is the transition from 2D towards 3D ultrasound imaging. 3D ultrasound images require a 2D transducer array that can steer an ultrasound beam in two dimensions. Such 2D transducer arrays are now made of small ceramic piezoelectric elements that all need to be addressed individually. The assembly of these 2D piezo-ceramic transducers is an extremely complicated and expensive process. This limits the usable size of medical imaging ultrasound devices.

The main objective of this project is to develop a flexible, large-area ultrasound technology for high-quality medical imaging and remote monitoring. We use thin-film technologies that were previously developed at Holst Centre for application in flexible displays. Due to economies of scale these technologies promise affordable fabrication costs, and in fact present the only realistic way to realize large (≥ 10 x 10 cm) and flexible ultrasound arrays. The large size of the 2D arrays will lead to higher image quality and much larger field of view. Integrated in the form of a wearable patch, flexible ultrasound arrays enable *hands-free* imaging, thereby reducing the physical burden for sonographers and improving the comfort of the patient.

Results realized

No.	Results planned	Realization
1	Technology roadmap for thin-film electronics integration	Yes. Detailed adaptations are expected in the coming years.
2	Fabrication and characterization of ultrasound medical imaging demonstrator	Yes. We have successfully demonstrated static imaging using an in-house fabricated 128 channel flexible transducer.
3	Report on imaging strategies and optimal transmitter/receiver partitioning	Yes. Ideas are elaborated on paper and using simulations. Two patent intakes filed in December.
4	Proposition development and setting up collaborations	Yes. We have reached out to different internal and external stakeholders to validate our business case
5	Strategic collaboration with at least two parties	Partially. We are setting up multiple collaborations with external parties.

Realized contribution to new knowledge and technology

We have optimized a thickness mode transducer which, unlike all other solutions available, is fabricated using an imprint and replication process that can be scaled to large area. The technology merges concepts from thin/thick film processing, display fabrication as well as nano-imprint technology. We extended our simulation framework from discrete element in air to arrays in water.

The performance of our thin-film transducers and readout improved by factor 4000 (!) since Jan 2020, to the level required for medical imaging.

Large-area ultrasound has a clear societal impact: it enables hands-free imaging for e.g. monitoring at home, which is a key enabling technology for the future organization of healthcare.

Realized contribution to the market position

We can offer feasibility study based on simulations verified with measurements on alternative transducer technologies. We offer patch integration studies, also using transducer arrays other than our (e.g. rigid CMUT and PMUT arrays).

Several discussions are on-going with companies (examples: Philips, Exo Imaging, Pulsify Medical) on technology feasibility studies, as a first step to commercialization. Once we have the first results of dynamic imaging on a tissue phantom, we plan to work together with strategic (clinical) partners (e.g. Erasmus MC, Radboud MC) to validate our technology in certain use cases.

4 inventions were submitted to the patent board of Holst Centre in 2020 (2 on fabrication technology, and two on compensation schemes to improve imaging of non-flat and stretchable arrays .

Publicity

Patent filings in 2020

PLT #	PD title	Inventors
2018110	Ultrasonic transducer with stacked membranes	Paul van Neer, Arno Volker, Hylke Akkerman, Gerwin Gelinck, Ton van Mol
2019093	Piezoelectric device with pillar structure and method of manufacturing	Laurens Peters; JL van der Steen, Roy Verbeek, Paul van Neer, Gerwin Gelinck

15 ERP Self-adapting smart batteries

ERP Contacts: Pavel Kudlacek (Project Lead), Peter Zalar, Gerwin Gelinck, Erik Hoedemaekers (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

The ultimate goal was to develop cost-effective and seamlessly integrated printed sensors in combination with state-estimation and control algorithms for battery systems. This program investigated and developed required building blocks and verified their performance in a demonstrator module comprising printed temperature, system design, and advanced battery control strategies. The research groups involved were TNO-Holst Centre and TNO-Automotive.

Commercial EV battery packs deploy single temperature sensor at module-level consisting of several 100 cells. Usually measurement is done at the main contact pad, which does not provide a detailed thermal map of the cells. Only when the whole module heats up to unsafe temperature does the system shut off, which is too late should the temperature rise be caused by failure of a single cell. Adding to this, the cell core heats up significantly more than its surface[3], which makes it vital to measure cell core temperature. Without detailed cell-level thermal information, individual cell state monitoring is not accurate. Moreover, as the state of the battery pack is directly dependent on the state of each cell, without accurate state-monitoring, pack degradation over time cannot be clearly monitored and battery capacity utilization will not be optimal.

The desired situation is a Smarter battery pack that is safer, faster, and can optimally store/supply more energy at the right time. Summarizing, detailed temperature information would provide:

- Earlier indication of cells that are over-heating (need not wait until the module is heated up)
- Up to 12% better utilization of installed cell capacity, via more efficient (and localized) thermal management
- Increased battery pack robustness and utilization of module capacity by turning off mis-behaving cells
- Clearer cell-degradation picture during operation, enabling better balancing, longer cell life and easier transition from 1st life into 2nd life applications
- Up to 30% faster and safer charging with anode-controlled charging

Following research topics must be addressed to develop commercially viable Smart battery pack with cell-level monitoring of temperature:

1. How to cost-effectively monitor temperature (and pressure) on cell level
2. How to accurately estimate the current status and future performance of the pack, (SoX – State-of-Charge, State-of-Function, State-of-Health)
    - Inaccuracy of state of the art SoX estimators is 5-10%; the ERP technology strives for < 2% inaccuracy
3. How to control and manage the battery system so that the sensed information is turned into tangible benefits for the battery system user or manufacturer
    - Up to 15% of cells' capacity is not utilized in state of the art packs; the ERP technology strives to close the gap to <3% of cell underutilisation and thus improve pack's total cost of ownership
4. How to implement the sensing and control technologies into a scalable battery management system

Results realized

No.	Results planned	Realization
1	A portable technology demonstrator primarily for showing at exhibitions	Realized and used during AABC exhibition. Furthermore, the realized cell-level sensing battery prototype can be used as a demonstrator.
2	> 12V and >0.5kWh battery pack prototype for evaluation of benefits of cell-level sensing and module-level control technology, including own testing BMS with:	Partly realized: Ad1) Yes, based on commercial temperature sensors. Improvement of damp heat stability of T

[3] Richardson et al.: *On-board monitoring od 2-D spatially-resolved temperatures in cylindrical lithium-ion batteries: Part I. Low-order thermal modelling*, J. of Power Sources, 326, p.377-388, 2016

	1) Cell level thermal state estimation (1K cell-to-cell temperature measurement accuracy; > 1Hz refresh rate; operational between 0-85% rel. hum., > 2 years cycle life) 2) Enhanced safety based on cell-level temperature sensing (overheating cells detection) 3) Accurate aggregated battery state estimation (<2% inaccuracy of SoC and SoH) 4) Control algorithms for faster fast charging (>10% improvement of the charging speed) 5) Control algorithms for cycle-life extension (>10% longer cycle-life) 6) Control algorithms for better cells' capacity utilization (>5% utilization improvement)	sensors realized too late to be implemented into the battery pack prototype Ad2) >10x faster detection of dangerous events compared with SotA. Ad3) Long term accuracy of SoH could not be evaluated as it requires lengthy testing. This activity will continue at TNO-Powertrains under development of remaining useful life and e-passport. Ad 4) Potential of 40% improvement in speed of fast charging demonstrated. However, the BMS algorithm has not been realized and its realization is linked to finding an industrial partner. Ad 5) Not realized and is expected to continue at TNO Powertrains under development of remaining useful life. Ad 6) Not realized as it requires cell-level control which was put on hold. Continuation of this topic is linked to finding an industrial partner.
3	> 12V and >0.5kWh battery pack prototype that allows development and evaluation of cell-level sensing and control technologies. Having the capabilities of the cell-level sensing module-level control prototype (Nr.2) and adding: 1) Capability to switch on/off call 2) Adaptive BMS with loss less balancing	Not realized: A concept of cell-level control has been worked out and its technical and commercial viability has been shown. The prototype has not been realized as the topic has been put on hold until an industrial partner is found.
4	Submission of at least one proposal for related EU funded project	Realized, E-Battres proposal submitted under LC-BAT-10
5	Visit of at least 2 exhibitions (AABC Europe, the second not yet identified)	Only AABC attended due to Covid-19 travel restrictions.

Realized contribution to new knowledge and technology

- TNO has acquired knowledge about battery system architecture, necessary building blocks, required accuracy of temperature sensors and implementation of sensorization into battery packs.
- A readout system for fast (>10Hz) reading of large sensors arrays (up to 1024 sensors) has been developed.
- The printed temperature sensor material formulation has been further optimized and resulted in improvement of the sensor's accuracy and stability under damp heat conditions. A technology for encapsulation of printed sensors has been successfully tested and encapsulated sensors have been proven to remain stable (<1% drift) under damp heat conditions.
- TNO has acquired knowledge on cell-level control architecture, potential benefits and development risks.
- TNO started development of battery pack aging (computer) model.
- Insight into the battery pack market and customers' needs has been deepened

The accuracy and stability of temperature sensors are important for other applications researched in 3F roadmap, e.g. sensors for car interiors. Their major improvement achieved in 2020 enlarges the sensors' valorisation potential also outside the ERP. Development and realization of the sensor read-out system will also be used in other projects within 3F roadmap.

The realization of the cell-level sensing prototype will help demonstrating benefits of TNO solutions but also opens possibility for future development of novel battery management algorithms and use cases at TNO Powertrains, e.g. remaining useful life, e-passport, used pack value estimation etc.

Battery pack computer model (not fully realized during the ERP) is expected to create a platform for development and validation of advance battery management algorithms, especially those targeting long term benefits. This will increase collaboration potential of TNO Powertrains.

The critical importance of creating a European industry along the battery value chain has been recognized up to the highest levels in the EC, in order to retain millions of jobs linked to ICE-based vehicles. Smart battery systems are part of the roadmap constructed by EU industry and the R&D community under umbrella of the EU initiative, Battery 2030+. A necessity to further develop cell sensing technologies to improve accuracy of battery thermal state estimation is explicitly mentioned in the Battery 2030+ roadmap.

Batteries are expected to play essential roles in the energy transition: (i) in the future intelligent energy system, creating storage to manage volatility & intermittency and optimize cost at all levels in the smart grid, and (ii) in electrification of mobility, as power source in electric vehicles. Indeed, batteries and smart battery systems have been identified as essential technologies for electrification in the 'Meerjarige Missiegedreven Innovatie-

Programma' MMIP9. With regard to KIA's, there are ample connections to MU1. Energie en CO_2 (energy storage, electric transport); MU6. Mobiliteit en Transport; as well as ST B. Geavanceerde Materialen; and ST F. Micro- en Nano-elektronica. For the sensor materials and devices, there are also connections to the roadmap of the High-Tech Materialen Topsector (HTSM); the smart, sensor-enabled battery system fits particularly well within the HTSM electronics roadmap

Realized contribution to the market position

From a business perspective, our proposed solution can enable several advantages that can lead to an increased market share, turnover and profitability of our partners. Therefore, it is expected to improve TNO's market position as well. These advantages are:

- Improve the performance of state-of-the-art battery packs, in terms of longer driving range and shorter charging times, by optimal management of cells.
- Enable cheaper battery packs, by virtue of being able to use cheap cells of mediocre quality without the need for over-engineering the pack for safety & performance.
- Disable defective batteries on cell level, by monitoring defectivities on cell level, the battery pack (depending on the balancing topology) may be used by switching off that specific cell without noticeable influence on the total battery pack capacity.
- More sustainable utilization of battery packs, due to better life-times because of avoiding cell abuse.
- Optimal re-use of cells for 2nd life grid-storage application, by accurate prediction of residual quality of the cells from the first application (EV).
- Shorter time-to-market, owing to reduction in rigorous pre-testing procedures, due to confidence given by the sensors.

The ERP team made the following efforts for establishing partnerships on various topics:

- *Unique-form-factor, printed temperature sensors.* We are discussing/have discussed this application with: a German Tier 2 automotive supplier (temperature sensors for batteries and electromotors), a Dutch sensor company (temperature sensors for batteries), two Japanese material/chemical companies (material for printed temperature sensors), and a US electronic OEM (temperature and pressure sensors for batteries).
- *Metrology system for battery pack R&D* – We are discussing/have discussed this application with: a Singaporean battery company, and a French automotive Tier 1.
- *Advance sensorization for battery packs* – We are discussing/have discussed this application with: a Dutch heavy duty vehicles OEM, a Singaporean battery company., SPIKE Technologies, effort is being made to contact a German car OEM in this regard.
- *Smart battery and advanced battery management* – We are discussing/have discussed this application with: the same companies as application 3 and a Japanese electronic conglomerate.

Furthermore, one EU project proposal, under LC-BAT-10, has been submitted and one trade show visited.

Publicity

- Report on concept of cell-level sensing technology (PPT)- internal
- Report on the stability and performance of the temperature sensors (PPT) - internal
- Report on benefits of cell-level sensing technology (PPT) – internal
- Value proposition and business development materials for 1) Printed temperature sensors for battery applications 2) Metrology system for battery R&D applications and 3) Advance sensorization for battery packs (PPT) - internal

16 ERP Appl.AI

ERP Contacts: Judith Dijk (Project Lead), Albert Huizing (Lead Scientist SNOW), Cor Veenman (Lead Scientist FATE) Hendrik-Jan van Veen (Science Director), Henk-Jan Vink (MD)
ERP Duration: 2019 – 2022

Progress 2020

Objectives

In recent years, significant progress has been achieved with Artificial Intelligence (AI) in conducting specialized tasks such as image recognition, natural language processing and games. World-wide, many investments are made in AI. This is also the case in the Netherlands, where institutes such as ICAI (Amsterdam), EAISI (Eindhoven) and collaboration programs such as the NL AI Coalition profile themselves with their specific instruments and programs. The fast developments in AI make it hard for any organization to keep up and apply effectively the combined set of techniques underlying AI. In this very competitive field a clear and defined AI proposition of TNO is required. Our Board has decided to concentrate TNO's efforts in an integrated program, called Appl.AI. TNO's ambition is to build on an already strong position and accelerate AI innovation through focus on integrational aspects of AI for complex task where safety and strict governance are at stake.

Within Appl.AI a research-oriented focus on generic technology and methodology development is combined with demonstration and development within use cases of our customers. Appl.AI is funded by ERP (Hybrid AI) and VP budgets.

To be able to apply AI in a responsible, explainable and controllable way a multidisciplinary approach is needed. In addition to domain expertise, also expertise from the fields of systems engineering, human factors, law, ethics and behavioral science is key to this approach. As a multidisciplinary applied scientific research organization TNO is uniquely positioned for this integration challenge.

Our research focuses on overcoming the significant shortcomings of current AI with respect to general purpose tasks, safe operations in an unpredictable world, interaction with humans and adherence to laws, regulations and ethics. TNO has a strong experience on approaching applied problems from a multidisciplinary and system integrator perspective. TNO has experts on generic AI topics such as advanced machine learning algorithms and symbolic reasoning and TNO has knowledge on expert-driven models in specific domains such as defense, mobility, health. There are other institutions that have capabilities on the individual components mentioned above, but within the Netherlands none has the combination of expertise in the various areas coupled with the domain expertise that TNO holds. It is therefore our ambition to extend our position on the system integration and architecture level for AI applications.

The mid-term objective for 2023 of Appl.AI is to develop capabilities that enable AI to be improved along the following four dimensions:

- *Environment:* from operations in a controlled environment to operations in an open world,
- *Purpose*: from specialized tasks to more general-purpose problem solving,
- *Collaboration*: from acting as a stand-alone tool to human-AI teaming,
- *Governance:* from applications where the governance of the AI can be permissive to applications where governance needs to be strict with respect to compliance with laws, ethical norms, and societal values.

Based on interviews we held with all science and market directors of the unit Roadmaps with AI as important enabler, we conclude that the research focus of Appl.AI is closely connected with the societal & industrial needs from the units. Moreover, the scope of the Appl.AI program fits with the long-term needs of the markets in which TNO is active.

An overview of the program is given in *Figure 10*. The program is structured around two integration flagships (which form the actual ERP), with generic research in the flagship projects itself and associated application centered research in use case projects. Commitment of external stakeholders in the uses cases shows their needs and is expressed through a multiplier on the research funds. In 2020 and 2021 several additional use cases are funded by the Ministry of Economic Affairs and Climate through the NL AIC.

The objective of the additional scientific exploration project is to perform research within the Appl.AI flagship objectives where cooperation with academic institutes and the Dutch Organization for Scientific Research (NWO) is stimulated. We aim to improve the academic quality and network of TNO by means of cooperation, publications and conference participation.

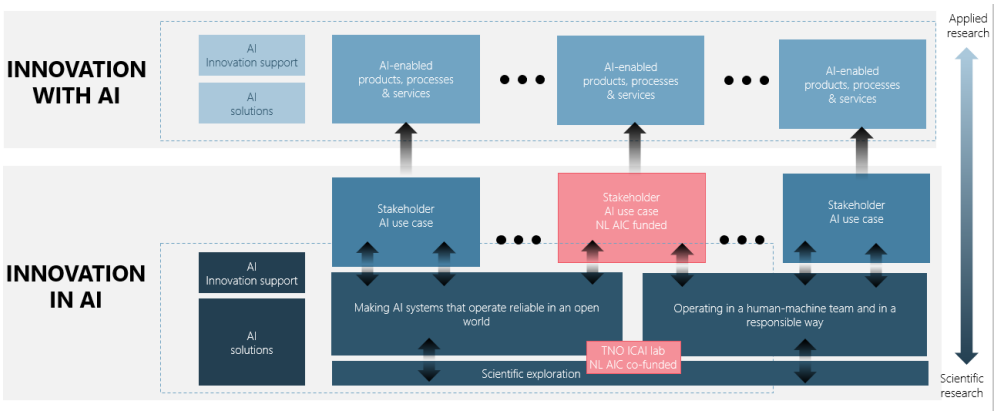

Figure 10: Overview of the Appl.AI program. For details see the text.

The two flagship projects that develop, integrate and demonstrate generic AI capabilities are:

- *SNOW:* Safe autonomous system in an open world
- *FATE:* Responsible human machine teaming in a dynamic world

These flagships address key topics for future AI applications in domains such as Health, Mobility, FinTech, Labor/Recruitment, Energy, Justice, Security, and Defense. The use case projects aim to co-develop AI technology related to the flagships in specific domains and to demonstrate the added value for these applications in operational context. The use cases of 2020 are presented in *Figure 11*. More information can be found in the Appendix.

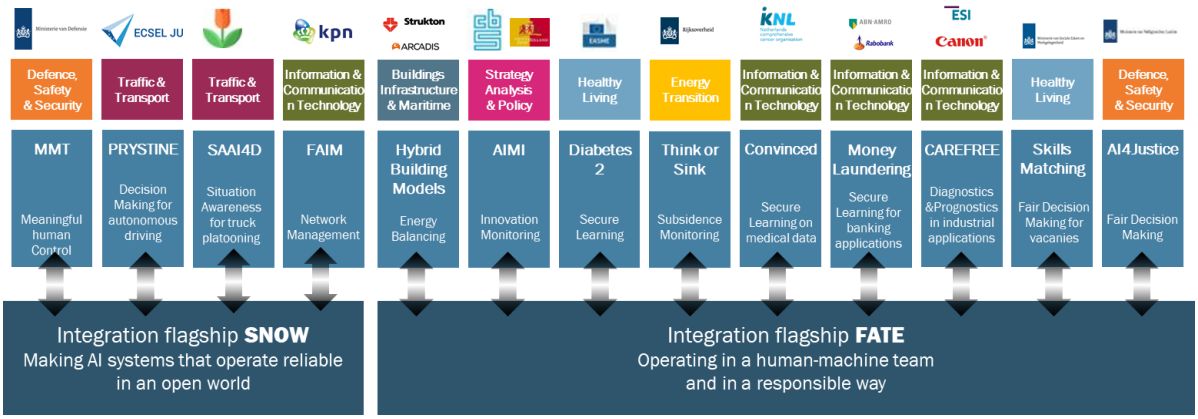

Figure 11: The Appl.AI use cases in 2020

SNOW

The objectives of the *SNOW flagship* project are to develop, integrate, demonstrate and evaluate AI capabilities for a self-aware autonomous system that can operate safely and effectively in an open world. Major elements of intelligence required for an autonomous system include an awareness of the situation, an awareness of the preferences of the user, and an awareness of its own capabilities and limitations.

For this aim we investigate methods and techniques that combine two different paradigms in AI: knowledge-based reasoning and optimization with data-driven machine learning, so-called hybrid AI.

The project focusses on

- AI techniques that enable understanding and explanations of novel situations in the external world.
- AI planning techniques that achieve the goal of the mission while satisfying operational, legal and ethical constraints in an open world.
- AI techniques that enable understanding and explanation of own competencies, and optimization of the system's internal configuration for a given task in a novel situation.

Overall, SNOW aims to develop the above AI capabilities on situation-, user- and self-awareness to increase the degree of autonomy of autonomous systems operating in an open environment. An increase in the degree of autonomy is achieved when fewer operator interventions are required in environments with similar complexity. The solutions developed will be implemented in a search and rescue use-case. Here we will keep track of several of Key performance Indicators (KPI's), such as the number of interventions in a particular environment (that is of measurable complexity).

FATE

The objective of the *FATE flagship* is to develop an expert assistant that acquires and extends its expertise through continuous learning from multiple potentially confidential and biased data sources and communicates its fair advices geared towards domain researchers, consultants and subjects. The ambition for 2023 is to build fair, transparent, and explainable (co-)learning: to develop and integrate AI methods for accurate and unbiased decisions, personalized explanations and justification of decisions, and continuous co-learning in human-machine teams . In order for AI to act as a meaningful partner in the fair hybrid decision-making process as described above, four important challenges are addressed:

1. *Bias-free data, learning, modelling, and prediction.* Current AI applications are built from large data sets generated by people. As people are not free from bias, the data they produce are not free from bias either. To prevent decision support systems from recommending people to make biased decisions, bias must be identified and mitigated in the automated decision process.
2. *Transparent and explainable learning.* The human and the AI participate in a continuous learning process, improving the decision-making for better achievement of the joint objective. The AI system must align its advices transparently with human expectations, (social) norms and values. To accommodate this co-act and co-learn process, AI must be able to both provide and understand relevant feedback and explanations to and from their human counterpart.
3. *Systemic effects in learning.* The collaborative decision making process creates challenges that arise in the long term, due to the feedback loop resulting from the continuous interaction between the AI system and the human collaborator. Together, the joint human-machine system, learns to improve its decision making process and the resulting outcomes.
4. *Secure learning* For this topic, the goal is to 1) identify the possibility of information leakage, given the approach that FATE has adopted and 2) how secure learning impacts the possibilities for Explainable AI.

Results realized

Program results

In 2020 we have shaped the Appl.AI program in its current form, by combining the ERP Hybrid AI, VP ICT/AI and strategic initiatives of the 2019 Appl.AI endeavor. All central activities with respect to AI are now aligned into one program. We have learned that the use cases indeed strengthen the research lines of the flagships. The different stakeholder groups are presented in *Figure 12*.

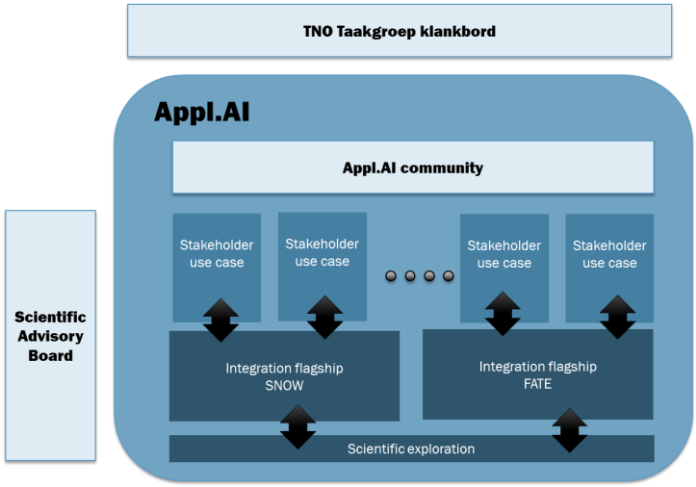

Figure 12: The different stakeholder groups of Appl.AI, visualized in light blue, and their connection to the program,.

We described the goals of Appl.AI in a position paper at the TAILOR workshop of the ECAI2020 conference. Due to the COVID epidemic we were not able to organize the planned Appl.AI event/ To position Appl.AI we therefore organized three webinars with more than 100 visitors each. The Appl.AI program was also presented in the “Snoek op Zolder” podcast of the NLAIC.

Collaborations

A collaboration has been setup with Fraunhofer IOSB. The objective of this collaboration called “Value-oriented Design and Enforcement for Responsible Automated Decision Making” (VALDERRAMA) is to improve the understanding of how AI algorithms can be employed as components in larger systems in a trustworthy manner across use cases in different application domains.

The project has a duration of 3 years and a budget of 1 M€ for Fraunhofer IOSB and 1 M€ for TNO. The TNO contribution focuses on goal functions and is materialized in the SNOW flagship project. During the kick-off meeting in November, opportunities for further collaboration between Fraunhofer and TNO have been identified in the area of automated driving, autonomous underwater vehicles, and AI engineering.

Within the Netherlands and the EU also other collaborations were setup and extended. In the Netherlands the most important ecosystem is the Netherlands AI Coalition (NL AIC). The current positioning resulted in a kick-start budget preluding the *Groeifonds* which we devoted to Appl.AI NL AIC labs and ICAI labs. Appl.AI will start five so-called NL AIC use cases financed from these funds. Next to that we received funding to systematically realize an ecosystem and work on data sharing technology. These initiatives are all step-up’s for the larger *Groeifonds* plans which will take shape in 2021.

Linked to the CLAIRE network the H2020 projects TAILOR and VISION were granted, were we work together with the EU AI network on defining the AI research agenda and proprieties. The connection to the EU AI PPP is established by the TNO member of the board of the BDVA (Henk Jan Vink) and by Freek Bomhof as member of a number of working groups. This will be continued in 2021 in the AI PPP or possibly the PPP from EU robotics.

The NWO project Smart Connected Bikes was granted, which aims at shared, real-time collaborative use of (sensor) data, wireless communication and Artificial Intelligence in new products and services. This will help to make bicycle-use more enjoyable, safe, reliable, and comfortable.

The DARPA Learning with Less Labeling (LwLL) program aims to make the process of training machine learning models more efficient by reducing the amount of labeled data required to build a model by six or more orders of magnitude, and by reducing the amount of data needed to adapt models to new environments to tens to hundreds of labeled examples. In this program 13 teams compete in solving these challenges. TNO is one of the two non-US teams in the program. In the first-year evaluation of the program TNO outperformed the other teams on the image classification tasks with low amounts of annotated data.

Scientific Exploration

To stimulate cooperation of research on AI with academic institutes in the Netherlands, AI related research from several research fellows and (assistant) professors are connected to this project, next to a number of PhD students and TNO employees working towards a PhD in close connection with TNO and different universities.

An overview of TNO professors, research fellows, lecturers and PhD students is provided in the appendix. An exceptional PhD student was Nadisha-Marie Aliman, who finished her PhD research and defended her thesis on December 2, 2020 after a period of two and a half year. In addition to 10 peer-reviewed publications at AI conferences and journals, the research by Nadisha-Marie is highly appreciated by the AGI community and she is ranked in the top 10 of influential AGI Safety researchers by Roman Yampolskiy an AGI thought leader[4].

SNOW

Within the set of desired AI-capabilities we developed real-time, hybrid AI software that integrates machine learning, a knowledge graph and symbolic reasoning. The integration of these individual results started with the definition of the SNOW-case: search for known victims in a villa that has caught fire and assist any found victims. The actual implementation of the SNOW-case in real-life required to integrate newly bought hardware (a SPOT robot from Boston dynamics with an additional camera, microphone array, speaker, mini-PC and e-bike battery) with the suitable set of software components, thereby creating our autonomous system called SnowBoy. The complete and actual SNOW-case was demonstrated in the last week of December in a real-life demonstration in which SnowBoy is tasked to search and assist victims in a villa on the premise of TNO.

For novelty detection we developed an ability to detect and characterize (novel) objects by integrating a taxonomy of object parts in either the learning process of a convolutional neural network (CNN) or in the classification process of a graph neural network (GNN). Training of the CNN with a taxonomy of body-parts was

[4] https://medium.com/@romanyam/2020-world-agi-safety-researcher-ranking-bda819247f03

used for detecting victims. Training of the GNN was used for detecting the type of room that SnowBoy is in based on typical objects one would find in such rooms (sink and oven in a kitchen).

For the characterization and explanation of novelties we automatically extract conceptual knowledge from online sources as ‘wordnet’ and ‘conceptnet’ to create a first, rudimentary taxonomy on concepts that should be known to the system as they are relevant for its operation. The approach was used to automatically extract the typical objects one could find in the rooms of a house, such as sink and oven in a kitchen, and so on.

For assessment of the system’s own competences an ontology on the system configuration (input, output and environment) is integrated with a characterization of the performance of each component by clustering internal measures of the input-output quality and of the environmental conditions using a continuous clustering approach. With this technology SnowBoy can understand when a visual detection of victims would perform bad (smoky conditions) and when not (clear conditions).

Planning a course of action for SnowBoy that depends on the context and user preferences has been carried out by integrating two developments:

- the capturing of prior knowledge about which action is preferred in which context in a knowledge-base, so that during operation only those actions relevant within the system’s current context are used for planning;
- the creation of a numerous plan alternatives via a Monte-Carlo planning process by combining such relevant actions one after another, and further optimize over each individual plan with a multi-objective utility function where the different objectives are weighed according to the user preferences as modelled by a Choquet integral.

In the demonstrator, SnowBoy can prune its possible actions to search in a room for victims using audio confirmation when smoke or bad light conditions were detected in the room, while SnowBoy can choose to plan a search using either visual or audio confirmation in other cases.

FATE

The FATE project focuses on development of an integrated decision support system that addresses bias and adaptive user involvement. This prototype is used to demonstrate the scientific progress. As use case the development of Diabetes- Type 2 for different age, gender, and social background groups was taken.

For bias detection and mitigation a model was developed that is aware of biases in the input data and takes them into account. The resulting general framework encompasses a comprehensive approach to bias management, including bias awareness, different bias mitigation strategies, and bias auditing. For the awareness, domain knowledge is used to identify the features related to the subgroups that may be sensitive to bias. A procedure has been designed to automatically detect whether or not bias will actually have an influence on the model performance.

Being able to explain a generated advice in a manner that is needed and understandable for the user is paramount. Towards this end, the prototype was developed such that it incorporates different manners of interaction for different types of users, such as subject matter experts (e.g. a healthcare professionals) and subjects (e.g. patients). In this system, the manner of interacting is tailored towards the particular needs of the users with respect to the type of advice that they seek. Additionally, hybrid models (combining knowledge and data-driven approaches) were explored with respect to their capability of arriving at improved predictions through the inclusion of domain knowledge, and their ability to generate explainable predictions by comparing the networks to other networks in similar cases. Trust calibration was explored through user experiences in which the impact of the mode of presentation by the system on user trust was examined.

In a changing world we would want a team of humans and machines that continuously learn from each other and positively reinforce each other in terms of avoiding unwanted biases and maintaining accountability. For this goal we developed interaction design patterns that describe adaptive techniques for adjusting the system behavior (type of explanations) to human’s behavior. Additionally, a first version of a user model is incorporated in the FATE prototype integrated system. Also, evaluation methods were developed for assessment of the system’s generated personalized explanations, including the modelling of their impact on the user’s trust in the system.

The secure learning approach was demonstrated in the Diabetes Type 2 use case. In such a use case an accepted way to work with sensitive data is to deploy federated learning. Recently, it has been shown that information leakage is a real potential threat in the case of Federated Learning. The threat analysis has been made specific for different types of users (honest-but-curious end users, and malicious end users). Quantification of information leakage has been identified as an open question; this is relevant when trade-offs between accuracy and information leakage are to be made. Other privacy preserving approaches like differential privacy have an impact on accuracy as well. In addition, bias identification and mitigation on distributed data has been identified as an issue.

Realized contribution to new knowledge and technology

A main characteristic of this program is its integral approach. The knowledge development in this program leads to concrete applications in different domains. The TRL steps from ERP to VP and finally to application are explicitly followed. This program will primarily focus on projects in line with its technology roadmap and the two integration flagships. Specific application aspects are addressed in other projects both within the program and TNO wide. Low TRL research is addressed in the scientific exploration project within the program, To large extent: our knowledge position regarding AI largely improves due to early research on the Appl.AI topics. Moreover, the position at academic institutes improves our technology position.

The relevance of the results for the governmental departments is discussed in the Appl.AI Taakgroup meetings. Some of the Appl.AI projects have governmental stakeholders, such as MMT (defence), skills matching (Social Affairs and Employment) and AI4Justice (Justice and Security). Next to that, they have access to the results of the other use cases and flagships as well.

In SNOW we extended our experience on autonomous systems by making an actual autonomous robot that can operate in a real-world without shortcuts in the demonstration as QR-markers for localisation or the detection of critical objects. The main portion of new knowledge was acquired in the software integration of SnowBoy, where we successfully integrated several state-of-the-art and newly developed AI modules in a complete, real-life robotic system. But, more importantly, that we created a Hybrid AI solution as every machine-learning module in the setup has some interaction with the knowledge-graph that is conducting symbolic reasoning. Sometimes this interaction is weak and one-way, yet for several modules this interaction between the two paradigms of AI is strong and cooperative for both components.

In FATE, we have shown cutting edge new results in several areas, such as bias detection and mitigation, using Graph Neural Networks in a Hybrid AI system for scene classification, generating explainable behavioural change advise (XAI) and exploration of design patterns on explainability and trust calibration.

In other areas, state of the art knowledge has been applied in order to arrive at an integrated system.

The main advancement of the FATE flagship, is that the research on the different topics (bias, explainability, co-learning and learning from confidential data) can be assessed jointly. The impact of biased data on explainability; the role of knowledge in trust calibration; the tension between transparency and secure learning. From various public interactions (e.g., presentations of FATE at international conferences) it becomes clear that such an integrated approach to various AI-related topics is rarely seen.

These developments put TNO in a good position to get to the forefront of applied AI; we intend to leverage this position internationally by building upon TNO's contributions in the H2020 VISION and H2020 TAILOR projects and newly required projects.

By bringing the ERP/VP together with the positioning of APPL.AI and with the ambition set out, the APPL.AI team has reviewed the strategic position of AI at TNO. The aim is to clearly carve out a fundamental and long term position of TNO in the landscape of AI developments. An exploration of the strategic goals of the units has been done in 2020. In 2021 a technology roadmap will be made, in which timelines and positions that we want to achieve along the way will be defined. This will also include proposing new Seed-ERP's and other investment programs to build a continuum of AI research in the coming 7 to 10 years.

Realized contribution to the market position

The Appl.AI program positions TNO towards top institutes, universities, government and other stakeholders with the broad research topics that TNO covers and the capability to apply them in sectors and use cases. Within Appl.AI use case projects are used to co-develop AI technology related to the flagships in specific domains and to demonstrate the added value for these applications in operational context. More information can be found in the Appendix

This way of working will attract new customers, attention and right to play in the research domain and with governmental bodies and with (potential) employees who want to be part of this endeavour. The connection with the roadmaps and PMCs in the units is crucial for this. The customers of TNO will have access to the total knowledge reservoir developed in the different flagship and use case projects. To be able to access this reservoir, the knowledge needs to be shared and explainable within the context of the TNO portfolio.

To position the Appl.AI program and TNO's AI vision a presentation for business development has been designed, in which both the scientific view as well as the market view are present. This presentation enabled the TNO business developers to present the Appl.AI program including the use cases tailored to their customer.

As a project SNOW directly received 75kEuro from the KIXS department of the Dutch MoD for supervising their trainees and employees in the combination of symbolic-driven AI with data-driven AI (machine learning). In

addition, the KMar has granted TNO a 150kEuro project related to SNOW for bringing AI-solutions to their SPOT robot.

Apart from those concrete market results the videos of the SNOW project have been shared by TNO-colleagues to external stakeholders. For example, Guido Veldhuis shared it with the TTCP panel and Pieter Elands has shared its results in TNO's 'Technology Radar Nieuwsbrief'. Also, they were shared by external persons to an even wider audience, for example, Tim Dykstra from Boston Dynamics with other SPOT-users and Daniel Crowe from GRAKN.AI within their community on focusing on knowledge-graphs.

Commercialization of the solutions developed in SNOW are typically initiated by the use-cases with which SNOW is cooperating within the Appl.AI program. These are Prystine, which is a European Project on automated driving, FAIM which is a project with KPN on the optimization of the electro-magnetic field surrounding a communication antenna, Human-Machine-Cooperating which is a project for the Dutch MoD on the delegation of tasks to an autonomous platform and CareFree which is a project between ESI and Canon on the self-diagnostics of printing systems.

The first year of FATE mainly positions TNO in a role related to applied AI. Although we can self-assuredly talk about topics like bias, personalized explanations, co-learning and the role of explicitly modelled knowledge in AI, the application that we are able to show is still relatively limited because it is based only on the Diabetes-2 use case. Interviews with all relevant other use case projects within appl.AI program have indicated that the FATE topics themselves are all relevant. We therefore expect that early commercialization of the results will be performed along the lines of the Appl.AI use cases.

Appl.AI has been strongly positioned in the National AI Coalition, NL AIC. In the various proposals and in the submission for the Kickstart budget, TNO and Appl.AI are mentioned as key enabler of AI in The Netherlands. As a result 15% of the funds of the initial Kickstart budget of NL AIC have been allocated to TNO, putting APPL.AI and TNO in a strong position for follow-up in the Groeifonds.

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--- APPENDIX – ERP Hybrid AI ---

An overview of the use cases funded by the Appl.AI program is provided *Figure 13*.

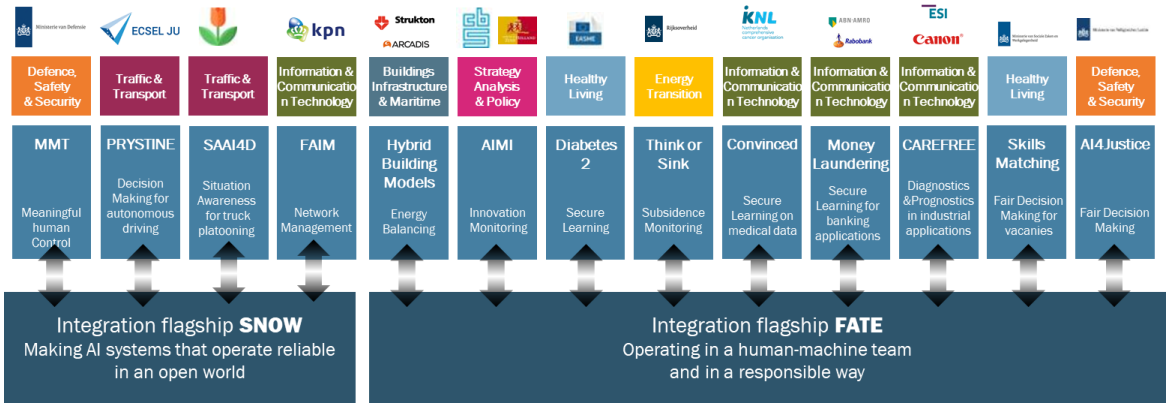


Figure 13: Overview of the use cases funded by the Appl.AI program

MMT: Man-machine teaming.

The aim of the man-machine teaming project is to develop meaningful human control: methods and algorithms that enable humans to keep control over autonomous systems. In 2020 the following results were achieved:

- A first design and implementation of a prototype was developed which allows delegation to autonomous systems in a simulated environment under meaningful human control;
- Two reference use cases were detailed defining a military operational and legal considerations behind meaningful human control which are used for scientific investigation.
- A testbed for measuring meaningful human control in a lab-setting was developed
- a philosophical basis of meaningful human control combining different ethical perspectives was drafted.

The MMT project is linked to SNOW as it develops methods and algorithms that enable humans to keep control over autonomous systems.

PRYSTINE:

Hybrid AI solutions for intelligent decision making based on knowledge and data applied in the autonomous driving case. This is a H2020 project with a large number of partners. The relation with SNOW is on the topic of control over autonomous systems in an open world.

SAAI4D: Situational aware AI for Automated driving

The goals of this project to develop an AI system that determines if an AI system is competent in the current situation and near future. This is tested in a truck platooning situation. In 2020 the following results were achieved. A previous developed intention predictor was retrained with a different dataset. The properties of the training dataset were described both symbolically (in the knowledge graph) and statistically. The ontology of the knowledge graph was extended to include unknown entities (unknown to the training dataset). Domain knowledge on the importance of entities in the knowledge graph was added. The reasoner was developed to combine the symbolic knowledge of the training set, the statistical description of the training set (to express doubt), and the importance of the entities with the observations of the current traffic state to express a level of competence of the predictor. Using the historical competence, a forecast of the future competence (in the next 2 seconds) was made with simple linear regression. The predictor and reasoner were implemented into an interactive dashboard for demoing purposes.

In the MCAS collaboration, we have worked with UvA to use ‘real’ observations of the traffic state (neural networks trained on simulated sensor output of CARLA) instead of idealized complete knowledge of the traffic state. This work is still in progress. With CWI, we are looking into the possibility of improving the forecast with graph neural networks. The link to the SNOW use case is that these technologies would enable sage and effective operations of autonomous systems in an open world, and would enable the self-assessment of the system in the current situation and context.

FAIM: Facilitating AI in mobile networks

The goal of the FAIM project is to develop AI algorithms for resource management in mobile communications networks. The goal is also to influence international 3GPP standards for 5G and beyond. This project is co-financed by KPN. In 2020 we achieved the following results. We selected beamforming as the Radio Research Management function and implemented a state-of-the-art Deep Learning Coordinated Beamforming for this application. We experimented with different explanation techniques for explanations of the input layer (how sensitive is the network to small changes in the input?), the hidden layers (which features are important in the decision making?), and the output layer (how can the output be translated to something human-interpretable?). This led to more insight on the potential and challenges of the introduction of AI/ML techniques in mobile network management, with a specific focus on the controllability, explainability and responsibility aspects.The relation between FAIM and SNOW is the lack of controllability and explainability in current algorithms due to which operators are very reluctant to use them in real-life.

Hybrid Scalable buildings

The aim of the Hybrid Scalable Buildings is to reliably predict short-term energy demand and supply of a cluster of multiple buildings. This is used for energy balancing. This project is co-financed by SMO funding, with stakeholders Arcadis and Strukton. In 2020 the following results were achieved

- A hybrid scalable model has been built that is generated automatically for different available databases on energy flows in the buildings. To this model AI based resident behaviour models are added.
- The predicted behaviour and sensitivity of behaviour on energy demand (using the physical model) will be used to explain to residents the effect of their actions on energy demand. For this task a federated learning method has been designed.

The link between FATE and Hybrid Scalable Building can be found in three aspects: 1) the applications of Hybrid AI by fusion of physical models and machine learning for the insight in energy flows, 2) explanations of decisions and 3) secure learning from privacy sensitive data.

Diabetes-2

The aim of the Diabetes-2 project is to develop secure federated learning and handling of biased data is used for building Diabetes-Type 2 prediction models. This project is co-funded by the H2020 project EASME and is aligned with the flagship FATE on these two topics. The Diabetes-2 use case is also used for the development and demonstrations in the FATE flagship. In 2020 the following results were achieved:

- Development of different approaches for bias identification and mitigation, and insight in the applicability in different contexts.
- For explainability, a systematic framework was developed which encompasses all relevant aspects of bias management, such as creation of bias awareness and tools for bias mitigation and auditing
- A state-of-the-art overview of Hybrid AI approaches for the healthcare domain, including an overview of the history of AI in healthcare, the current approaches, missing pieces, opportunities for the (near) future, and implications for transparency, explainability and trustworthiness when using this approach.

Think or Sink

The aim of the Think or Sink project is to develop a hybrid AI data and model for the entire Netherlands with a special focus on the northern gas field area of the Netherlands and the Green Heart. This project is co-funded by task SMO from the ministry of Environment. In 2020 the following results have been achieved:

- A hybrid AI data and model workflow for subsidence predictions has been developed based on (1) intermediary outputs generated by the pure physic-based approach and data from geodetic measurements
- An explainable AI module has been developed that can explain the feature importance on the outcome and provide local and time-series explanations.
- A Bayesian physic-based approach was enriched with two new modules. One module to handle the deep subsurface data provided by Vermilion Energy. One module to handle the shallow subsurface of both GeoTOP and groundwater tool.

This project is related to FATE on the topics of explainable AI and federated learning to enable the use of confidential data.

Carefree

The project of Carefree is an application of hybrid AI in industrial processes for maintenance purposes. This project is co-funded by Canon (CPP). In 2020 the following results were achieved:

- the feasibility of AI-based diagnosis within the industrial application domain was demonstrated by means of several prototypes for a part of the machine. We pursue a hybrid-AI approach where the core

of the reasoning engine is a Bayes net modeling the machine and required probabilities are learned from machine data.
- We took first steps in developing a scalable technology where we can automate the creation of the reasoning engine based on system-level descriptions. This demonstrated Bayes as a valid basis for system level reasoning and demonstrated that it forms a scalable approach towards diagnosis of large industrial systems.
- We have analyzed data sets of machine failures as input for a learning process and have concluded that a pure data-driven approach will not suffice. This supports that we need our hybrid-AI approach.
- Together with CPP we did a first experiment to integrate the approach in the CPP system engineering methodology. This delivered another prototype which will the basis for a study on the requirements for System Level Modelling activities at CPP

This project is related to both SNOW and FATE on the topics of self-assessment and explainability of the condition and performance of complex equipment.

AIMI: AI for monitoring innovation

The project AIMI has as goal to develop a hybrid (AI / expert-driven) approach for an innovation monitor that can recognize, monitor and project innovation trends on the ecosystem. This project is co-funded by the Province of South Holland. In 2020 the following results have been achieved

- the information need and user requirements for the information dashboard are defined
- a knowledge graph, a first version of a metadata standard and a database for the topic AI are developed

AIMI relates to FATE on the topics interactive knowledge modelling and the generation of explainable statistics.

Convinced

The aim of the Convinced project is to developing AI for data from different parties such as IKNL with secure data sharing technology. This TKI project is funded by IKNL and CZ. In 2020 the following results were achieved:

- New solutions are developed to analyze vertically partitioned data without compromising the patient's privacy using Multi-Party Computation (MPC). In particular this project focused on survival analysis: an often-used technique in oncology data research that can be used to indicate how likely someone is to be alive a few years after diagnosis. Additionally, it can give insight in which characteristics might relate to the chances of survival.
- It has been shown that MPC can indeed be employed to perform survival analysis on vertically-partitioned data, without having to reveal any sensitive data. For some survival analysis techniques this can be done while keeping the performance of the secure solution high enough for practical application on realistic data sets. For more complex survival analysis techniques additional research is needed to improve the performance before it can be applied in practice. Follow-up steps to bring the developed solutions towards operational applications have been identified.

The link to FATE is on the topic of secure learning.

Money Laundering

The Money Laundering project focuses on collaboratively detection of money laundering with scalable secure learning models This is a TKI project with the Rabobank and ABN-AMRO as financing partners. In 2020 a new algorithm for risk propagation is developed based on transaction data using Multi-Party Computation.

The link to FATE is on the topic of secure learning.

AI4Justice

The aim of the AI4Justice project is to solve self-fulfilling prophecy & tunneling in high impact applications. Solutions should be: Explainable, Fair, Legal, and most importantly… stand in court. This project is co-financed by the Dutch ministry of Justice and Security. In 2020 the following results are achieved:

- the fundamental reasons for 'tunneling' and 'self-fulfilling prophecy' to occur
- have been explored, and a set of (algorithmic) rules have been determined in which the effects of 'tunneling' and 'self-fulfilling prophecy' can largely be diminished.
- A first version of a booklet was made with interviews with pivotal persons in the domain to collect their opinions on the ethical and societal consequences, restrictions and limitations of using pre-trial risk assessment tools.
- Prototype software has been developed and installed at a DoJ location to derive the probability of someone getting 'onvindbaar', however it is also monitoring the effect of various visualizations, complexities and the understandability. The latter by means of introducing intentional mistakes, and checking if the subject detects those.

The link to FATE is on the topics bias mitigation and explainability.

Skills matching

The goal of the skills matching project is to develop technology to improve the matching between vacancies from companies and job seekers. This project is co-funded by the UWV. This project is executed in collaboration with CBS. The results of 2020 are

- The development of a connection between the CompetentNL ontology and the O*NET skills taxonomy from the US and a first rpoof pf principle of automating the alignment process of the CompetentNL ontology with other knowledge bases by applying Natural Language Processing (NLP)
- The setup of a first software architecture and a roadmap towards achieving dynamic ontologies
- The development of an explainable skills-extraction module and an explainable vacancy-scoring methodology consisting of a vacancy classifier, skills overlap and bias modules.
- The realization of a TRL 4 demonstrator and interface for interaction with AI functionalities for skills extraction, matching of vacancy texts and bias assessment, including textual descriptions of the project and its elements.

The link to FATE is on the topics of bias determination, bias explanation and bias mitigation.

--- END: APPENDIX – ERP Hybrid AI ---

17 ERP Decarbonisation

ERP Contacts: Pascal Winthaegen (Project Lead), Dick Koster / Ardi Dortmans (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2019-2022

Progress 2020

Objectives

The (inter) national climate guidance and objective

The causal link between the exponentially increased CO_2 emissions in the last 100 years and the accelerated global warming since then has been convincingly demonstrated. Worldwide, governments and the business community have increasingly formulated objectives and measures to limit and, if possible, reduce the emission of greenhouse gases and associated effects on the climate. In the Netherlands, this has recently led to the formulation of the government's ambition to reduce greenhouse gas emissions at a national level by 49% by 2030 and by 90% by 2050 compared to 1990.

Share of the Dutch chemical industry

Given the geographical location and associated good supply and export possibilities, there is an above-average high concentration of large-scale chemical industry in the Netherlands. With the associated use of energy and fossile raw materials for the production of basic plastics and artificial fertilizer, the chemical sector in the Netherlands, when compared to most other countries, makes a relatively high contribution to the total national emissions of CO_2 and other greenhouse gases such as N_2O.

In Limburg, the share of the chemical industry, located at the Chemelot site near Geleen, in the total energy consumption and the emission of greenhouse gases is even greater. The energy use and associated emissions amount to about 30% of the total of the province and represents one of the largest CO_2-emitting energy consumers on a national scale. Securing the "license to operate" of the companies active at Chemelot and the associated continuity and growth of economic activity, employment and broader social relevance, represents an interest that exceeds that of the site, region and province of Limburg. However, the province of Limburg has taken the lead in embedding the foreseen Chemelot transition in a wider response (Het Limburgs Aanbod) to contribute to the national climate agreement goals, and has and is willing to provide structural funding to make them become a reality.

The ambition of Chemelot

Compared to other chemical sites, the activities of the various companies operating at Chemelot are largely integrated. The various independent companies that originate from the former DSM activities make use of joint infrastructure wherever possible, which is centrally maintained and further developed by Sitech Services BV. The location Chemelot and active companies therefore provide an environment and partner base with a special potential, compared to other chemical sites in the Netherlands and Western Europe, to realize "Climate Proof Chemistry" in a field lab on industrial scale.

In response to the climate targets formulated by the government, the six largest and energy-/emission- intensive Chemelot-based companies have drawn up a concrete proposal in April 2018 to enable Chemelot to develop into the most sustainable and competitive chemical site in Western Europe over the next 10 years. This proposal has been drawn up by a jointly formed Chemical Sustainability Team (CST) which, under the direction of Sitech Services BV, has integrated an inventory of the various emissions and options available to Chemelot in order to reduce them through process greening.

Brightsite

In order to achieve this the "greening" of the Chemelot site and provide an international leading example on the basis of which access to additional national and international funding sources will be possible in the appropriate frameworks a new initiative was required. To this matter, the Brightlands Chemelot Campus organization, providing an open knowledge development environment adjacent to the Chemelot Industrial site, has proposed TNO, Sitech Services and the University Maastricht to join forces in a new shared research, development and implementation oriented Brightlands Sustainable Technology Center at its premises. Following a preparative phase, a formal Consortium agreement to establish the center has been signed on June 25th, 2019, under the name “Brightsite”.

In the above mentioned " Limburgs Aanbod" the establishment and provincial support for Brightsite is already foreseen. On a national scale, the Brightsite initiative can be linked to incentive programs which are made available by the Dutch government to achieve the objectives of the climate agreement. In this context, Brightlands Chemelot Campus already fulfills an important intermediate position in by coordination of the so-called “Trilateral consultations” in which, with the support of the Dutch, German and Belgian governments and with partners from industry and knowledge infrastructure, work is being done to set up and implement a cross-border agenda for greening of chemical sites such as Chemelot. Due to the timely start-up of Brightsite with the support of the Province of Limburg, Chemelot with an international partner base it can take the lead in addressing the global emission challenge of the chemical industry as a stepping stone for innovation and application of new technologies. By this initiative the application of climate-proof Chemistry on industrial scale can become a reality by 2050.

TNO has the ambition to play a leading role in Brightsite by developing technologies and knowledge which support the scale up of (process) technologies that ultimately make the greening of chemical campuses like Chemelot possible. The market and technical scope of Brightsite closely interacts with roadmaps of the units Industry, Circular Economy and Environment and ECN part of TNO.

Brightsite will focus on a number of transition programs that are energy, circularity & alternative feedstock, system integration and process safety related. During the initiation phase and the startup of Brightsite, the priorities were defined in close relationship with the partners and the associated industry. In order to provide financial and operational working space to play the appropriate envisaged TNO part in the realization of the overall decarbonization goals of Brightsite, the present ERP has been set up.

The following Brightsite program lines are defined:

1. Reduction of emissions by electrification	**2. Reduction of emissions by reduction of naphta and gas usage**
1a. Electric high temperature heating 1b. Plasma activated cracking & decarbonisation of methane 1c. Molten metal decarbonisation of methane 1d. Sourcing, transportation and storage of electricity	2a. Gasification of plastic, domestic waste and biomass 2b. Pyrolysis of plastics 2c. Dissolution/depolymerisation of plastics 2d. Conversion technologies of biomass streams
3. In-/post-process emission reduction	**4. Securing integral process safety and societal acceptance**
3a. CO_2-Capture/Storage/ Use (CCS/CCU) 3b. Reduction of N2O-emission 3c. Use of residual heath	4a. Safety Leadership 4b. Governance & processes 4c. Asset design & operations
5. Transition scenarios and system integration towards 2030-2050	**6. Education and human capital**
5a. Modeling of the Chemelot site and its connections to the outside world 5b Outlooks for developments external to the Chemelot site 5c. Stakeholder engagement	6a. Bachelor of Science Circular Engineering 6b. Master of Science Sustainable Manufacturing 6c. Master of Science Biotechnology
Scouting of new technologies will be part of every program line.	

The following research topics were addressed in Brightsite ERP Decarbonisaton- research lines:

1.Reduction of emissions by electrification

In the so-called cracking process at Chemelot and similar industrial chemical sites, petroleum-derived molecules are broken down from so-called naphtha oil into smaller molecular units to obtain raw materials for polymers. Natural gas is currently being used to achieve the required temperatures. The cracking process is therefore one of the largest sources of CO_2 emissions at Chemelot. If the required temperatures could be achieved sufficiently stable and homogeneously by means of electrical heating and if sufficient renewable electricity is available for this purpose, a large contribution could be made worldwide to achieving the climate targets. In view of the worldwide application of the current cracking technology and the billions of investments involved in replacing it, international partners outside of Chemelot are already interested in participating in a Brightsite shared research program.

Electrification of currently heating technology based on fossil fuels can, if applicable on an industrial scale, make an important contribution to the achievement of climate targets 2030-50. However, the required electrical energy

must then be available from sustainable sources and in the necessary quantities and certainty in order to be able to realize the envisaged transition. In this Brightsite program line, the current and expected availability of existing and possible future sources of electrical energy will be mapped. If the studies appear to be justified and there appear to be suitable technical possibilities and positions, from this program line development activities can also focus on the local generation of sustainable electrical energy to reduce the dependence on external sources.

CO_2 is also formed in the industrial production of hydrogen from natural gas. Using alternative "decarbonisation" methods, it is in principle possible to decompose methane into carbon and hydrogen without CO_2 formation. In particular, the decarbonisation by means of plasma activation and conversion at high temperature in liquid metal offer the possibility of new technologies to be applicable on an industrial scale. The potential of this and other decarbonisation options will be investigated in Brightsite framework through feasibility studies involving external knowledge partners and, if there is a potential presence on a practical scale, will be further developed and applied.

2. Reduction of emissions by reduction of nafta and gas usage

A chemical site such as Chemelot has a significant consumption of fossil resources as feedstocks and fuels (e.g. a precursors or in heat generation). At the Geleen site, naphtha and natural gas are the two largest fossil resources. To achieve the climate targets of 2030 and 2050 there is a need to identify how fossil resources can be replaced with other (e.g. renewable) sources. In this program line, the use of biomass and plastics will be considered in this context. Both streams are deemed to be available in various quality (i.e. separate) streams and also as combinations of both biomass and plastic (e.g. Refuse Derived Fuel (RDF), Municipal Solid Waste (MSW) and Solid Recovered Fuel (SRF)).

The program line will address the required technology development (and associated assessment) that will underpin the economic and sustainable conversion of biomass and plastic waste into feedstocks for the (future) Chemelot site, in turn reducing fossil feedstock consumption and CO_2 (and equivalent) emissions in Scope 1, 2 and/or 3. This program line will evaluate and generate technology options for technology demonstrators first at Chemelot and next elsewhere, while program line 5 is integrating these into site and national/EU context. Brightsite founding partners incl. TNO has the ambition to develop knowledge and technologies and develop a Brightsite center and field lab for demonstration. The following sub programs have been identified:

2a. Gasification of plastics, domestic waste and biomass
2b. Pyrolysis of plastics and biomass
2c. Dissolution/depolymerization of plastics
2d. Conversion technologies of biomass streams

Within the program, sublines 2a and 2b will identify and evaluate the use of gasification and pyrolysis technologies for the conversion of biomass (residues) and waste to suitable output for the substitution of naphtha and natural gas. Gasification processes convert biomass, plastics or mixed streams at high temperatures to oil, lighter hydrocarbons or synthesis gas depending on temperature and operating conditions. Gasification could provide solutions for various processes at Chemelot: hydrogen production for ammonia (OCI), Urea, melamine, caprolactam, acrylonitrile, CO2, ethene, benzene, BTX. Pyrolysis of plastics and mixed waste streams produces gas, oil and coke fractions. This oil fraction could be suitable as feedstock for the naphtha steam crackers at Chemelot. Subline 2c focuses on chemical recycling of durable plastics found in electronics, automotive and construction. The program evaluates solvochemical recycling technologies to access the additives for removal prior processing. Additionally, condensation polymers by dissolution and depolymerization followed by purification of the monomers. The most relevant plastics considered for the Chemelot site is Geleen are: polyamides (PA 4,6 and PA6, DSM Engineering plastics, Fibrant), polyesters (PET, Ioniqa) and polyolefins (PP, SABIC, Mitusi and QCP). Assessment of PVC recycling (Vyonva) is also a potential program item. Finally, program line 2d deals with a number of conversion technologies to valorize biomass streams. This item was added later in 2019 and initial scope is to inventories biomass streams and potential conversion technologies in relation to potential future new value chains for Chemelot.

3. In-/post-process emission reduction

By reusing CO_2, process chains can be connected to each other and possibly closed completely circularly. On a limited scale circular recycling in the horticultural sector is already possible at the moment, with CO_2 being re-established in plant material. If sufficient and adequate cost price is available from sustainable generation, electrochemical or plasma-activated reduction of CO_2 to make chemicals is a realistic future option. For the time being, however, the surplus of CO_2 will have to be collected, stored and / or disposed of in a responsible manner. Within this program line, Brightsite will be able to translate available and new techniques that are available for this into application scenarios for the short and longer term and where appropriate development and application of new technology will be implemented.

N_2O is formed as a by-product during the production of nitric acid and fertilizer based on it and, like CO_2, is a greenhouse gas, but with a 265 times stronger effect. Reduction of N2O emissions therefore contributes

relatively strongly to the achievement of the total emission target of chemical sites where ammonia is produced. A substantial reduction in N2O emissions has already been achieved at Chemelot through the application of new techniques in the past 15 years. However, it is also clear that for the time being few additional possibilities for further reduction are available. In this area, new options will be explored from Brightsite in collaboration with suppliers and developers of currently used industrial catalysts to overcome current limitations.

Regarding the reduction of CO2 emissions on an industrial site such as Chemelot, there is still much to be gained in principle if the residual heat present at various locations can be reused efficiently. Conversion of these mostly low-temperature heat flows to high-temperature energy is therefore a requirement that can be realized on an industrial scale with heat pump technology specifically developed for this purpose. Linked to this are technologies for efficient heat storage to stabilize temporary surpluses and shortages. In the Brightsite framework, both the application and the development of these two technology lines will be able to take shape. The use of residual heat in the built environment is already an ongoing project in the Het Groene Net, with which residual heat from SABIC is supplied to the district heating of Sittard-Geleen.

4. Securing integral process safety and societal acceptance

Process safety and societal acceptance are of continuous concern among the global chemical industry. An organization's implementation of safety and communication programs directly affects its reputation, profitability and ability to attract and retain talent. Ineffective safety programs can have severe repercussions for those responsible for protecting workers and society.

The development and introduction of new technology and energy resources, as required for the achievement of the climate targets 2030-50, can only take place on an industrial scale if (process) safety is secured and social acceptance is taken into account.

The objective of WP4 is improvement of the process safety performance and to enhance societal acceptance in complex (industrial and high tech) systems. Therefore, WP4 will develop data-driven technology by research (and application) of predictive analytics and combining data from different sources. Key research includes application of predictive analytics, creating insights in complex systems and utilization of data (from multiple sources) into data driven technology.

5. Transition scenarios and system integration towards 2030-2050

The application of eligible new technologies on the basis of which the realization of the climate targets 2030-50 will ultimately become possible on an industrial scale can only occur if the integral quality, efficiency and safety of the existing and future production processes can be guaranteed at every transition step. For Brightsite, Chemelot is the practical testing ground for this, but the far-reaching integration of infrastructure and the linking of primary and supplying production processes requires that there is constant certainty about the effects that will occur at the site level when implementing new technology. In view of the different development and implementation periods of the various new technologies, scenarios will be drawn up for possible application of sub-technologies in this program line. To this end, available models will be further developed to identify the effects of new technology in a digital "twin" environment on the basis of available and expected process information. On the basis of this, it will be possible to determine in advance at what period which sub-technology can be applied responsibly and efficiently.

For Chemelot and similar chemical sites, the stable availability of sustainably produced electricity, raw materials such as hydrogen and pyrolysis oil, as well as the removal of captured CO_2 is a key factor, but also a potential breakpoint for the timely realization of the emission targets. For the intended integrated approach, Brightsite will map out in more detail what can be realistically expected in the short and longer term to be applied on an industrial scale. From this, scenarios will be opened in the Brightsite framework for adaptation and renewal of the logistical and infrastructure aspects related to location level.

The program line deals with the dilemmas, hurdles and (collateral) risks on the one hand and site- or cross site societal synergies and new opportunities on the other hand, all associated with future successful implementation of newly developed technologies on a complex chemical site like Chemelot. The integral safety, quality and efficiency of the existing and future production processes need to be guaranteed at every transition step so that the competitiveness of the site is maintained.

6. Education and human capital

In order to ensure appropriately educated human capital to investigate, develop and apply new climate proof chemical technologies and supporting activities, new generations of students at various education level are required. The development of an education curriculum for this is the key role of the University of Maastricht next to the execution of academic research at low TRL. Results and outlooks resulting from the TNO involvement in the former Brightsite program lines will provide input and content for this.

New technology scouting

The above described program lines have been selected and detailed in view of the expected possible contributions to reduce emissions in the timeframe 2030-50. However new and sometimes possibly radical emerging technologies are emergent and will become available in the future. Brightsite will have to proactively identify and assess such new technology in view of the possible impact and applicability and expected price-performance when applied on a practical scale at sites like Chemelot. Clearly this program line will be executed by TNO in close interaction with University of Maastricht and associated appropriate (inter)national academic and knowledge institute partners.

Results realized

No.	Results planned	Realization
1-1	Report on experimental and numerical cracking optimization Report on on demo plant design and analysis of electrified cracking process chain	No, due to shift in priorities in WP1. Instead TNO report (Word document): Feasibility study Electric naphtha cracking, review paper: Electric cracking of hydrocarbons
1-2	Powerpoint presentation on approach how to improve Hüls process	Yes, Word document with research questions and experimental approach
1-3	Powerpoint presentation on other plasma routes: results of literature study, plasma simulations, and plasma source development	Yes, powerpoint on literature research Plasma simulations started but not finished Plasma source development started but not finished Several proposals submitted for additional funding (1 granted, 1 pending (expected jan 2021), 1 investerings fund pending
2-1	Opportunity framing Milena/Olga demonstration: Identify phase Assess-phase Select phase	Identify phase: Yes Assess-phase: No, not completed in 2020 (due Q1-2021), concept report per email (December 2020)
2-2	Presentation on pyrolysis companies, TRL to SABIC If positive, screening of pyrolysis experiments and technical due diligence TEA support	Presentation: Yes, pptx No follow-up Extra: Torwash technology developed, powerpoint
2-3	Presentation PA-6 proposal to Fibrant/DSM EP based on 2019 study based on literature review Proof of concept of catalytic depolymerisation and establishment of participation/support of at least one site user (Q2/3) Basis for catalyst proposition as supported by process design to be elaborated further into BrightSite programme (Q4) PVC Vynova follow-up and plan for PVC recycling, hydrodechlorination	No. No follow-up, due to COVID-19 and lack of real interest
2-4	Results Torwash known and communicated Plan for biomass routes developed and presented to CST: literature study, high level TEA and link to TNO units and new/current site users	Torwash presented, transferred to Brightsite-PL3 Plan and literature study developed and presented (pptx)
2-5	LCA matrix support to WP5	No (integral in WP results) Extra: Collaboration established with Utrecht University (prof. Weckhuysen) on liquid-phase pyrolysis
3-1	Selection of one target chemical to be produced on the basis of CO2 and applicable and synthesis routes. Critical overview over CO2 capture options for the major CO2 emissions.	Meetings with Chemelot companies. Draft CCU White paper.
3-2	Alternative process option with intrinsic less N2O formation for caprolactam production.	Meetings with Chemelot companies. Interest from AnQore for catalytic decomposition. A four-way NDA with AnQore, Shell (licensee of TNO catalyst) and Sitech.
3-3	Identification of at least one integrated demonstration location for a heat pump with at least 2 MW power rating. 5/2020 WP3-X • Definition and assessment of one use case for start-up digitization at Chemelot • Identification of at least one breakthrough energy efficiency measure 5/2020	Interest from Vynova and Arlanxeo in the technology. Despite multiple interactions no follow up.

3-4	Definition and assessment of one use case for start-up digitization at Chemelot • Identification of at least one breakthrough energy efficiency measure	Residual gasses: Due to other priorities, no further steps will be taken in the coming years by site-users. Digitization: Promising virtual multi-party Front End Loading session meeting held.
4a-3	Report. Development of Early Warning System	Yes (final draft)
4a-4	Literature study. New and societal options	Yes (first draft)
additional	Brightsite presentation. An introduction to HSE management in era of AI	Yes
additional	Brightsite leaflet. HSE management powered by AI	Yes
5-1	Modeling software selected and purchased	Yes
5-2	Second generation modeling system that provides insights on the mass and energy balances of Chemelot	Yes Chemelot Integrated Model System; A tool to assess future pathways Chemelot Integrated Model System; Model description and base year (draft) Scenarios for developments in the outside world (draft)
5-3	Input for infrastructure decisions based on modeling and stakeholder involvement	Yes Workshop e-markten
5-4	Assessment of technologies on request of the site users in cooperation with other program lines, including stakeholder involvement	Yes Methodiek voor allocatie van productiekosten voor technologie die één of meer van de producten van de naftakraker produceert Workshop Sustainable products for Chemelot Report Melamine case

Realized contribution to new knowledge and technology

1 Reduction of emissions by electrification

Together with the partners a deeper insight on the business case of plasma chemistry has been developed. Part of this is an economical calculation model for a complete plant and the required investments and expected profit. A start has been made with simulation of high pressure plasma's, which is a unknown field in plasma simulations. This will be of benefit on the engineering and design of a full size plant. Design of experimental test setup realized to provide feedback on simulations and pilot plant design.

2 Reduction of emissions by reduction of naphtha and gas usage

New knowledge has been developed in the field of technical integration of thermal cracking on-site of Brightlands Chemelot Campus. Several options have been investigated and weighted according to OPEX, CAPEX, safety, risks, etc. In addition, innovative plastic waste pretreatment technology has been developed, based on previously developed Torwash® technology. This has large potential to broaden the potential feedstock to be used in pyrolysis processes, relevant for three (future) site-users (next to SABIC). Finally, new concepts have been investigated for liquid-phase pyrolysis of olefins, for highly efficient recycling of food-contact packaging materials.

3 Process innovation

New knowledge has been obtained on the application of CCU for the Chemelot site. New emerging technology pathways have been identified, and a preliminary review has been adopted.

4 Process safety and societal acceptance

A first working (AI-powered) predictive model ("Safety Stethoscope") for enhancement of process (safety) management is available at TNO's DIAMONDS-platform. The model executes advanced data analytics and identifies hidden patterns (including correlations and associations) in large amounts of unstructured data. The rudimentary model has proven to ready for development of an advanced AI-powered EWS-system in the era of Industry 4.0, able to identify anomalies in complex systems, derive predictive values and to predict (major) disruptions and/or incidents (in order to detect and stop them from happening).

WP5 Transition scenarios and system integration towards 2030-2050

The Chemelot Integrated Model System (CIMS) that has been developed optimizes against various scenarios for e.g. electricity prizes and CO_2 prices. The developed transition paths will help site users to define non regret options and investments. The insights are essential for positioning Chemelot in the national and international discussions on for instance infrastructure. The methodology that has been developed can also be used in other industrial clusters.

Realized contribution to the market position

1 Reduction of emissions by electrification

In WP1 a strong collaboration with Maastricht University (prof G. van Rooij) has been established, together with the university a dedicated plasma lab will be realized on the Chemelot site. In the submitted proposals strong collaboration with the Brightsite partners Sitech, Brightlands Material Centre (BMC) and Maastricht University has been established. Other site users of Chemelot like Sabic, OCI Nitrogen and DSM cooperate in the MOOI proposal. We are actively seeking connection with potential suppliers of equipment to become part of the research program as well as potential users of the technology outside Chemelot. In the NOW perspectief proposal companies like Shell are actively involved. Initial discussions regarding this topic have been started with Borealis, Evonik, Monolith and Transform materials

2 Reduction of emissions by reduction of naphtha and gas usage

The results on use of biomass and plastic waste as circular feedstock to reduce naphtha and natural gas usage have drawn the attention of site users and scale-ups. A MOOI proposal has been submitted including the important topic of feedstock pretreatment. Furthermore, activities on chemical recycling have been incorporated in the Green Deal proposal EUROBOROS, initiated by the Brightlands Chemelot Campus site-users. Discussions between scale-up Synova and site-users have been facilitated, potentially leading to a demo-facility at BCC. The application of chemical recycling has been thoroughly evaluated for several feedstocks and site-users and deemed interesting. Furthermore, a collaboration with Utrecht University has been initiated on third generation chemical recycling technologies "liquid phase pyrolysis". In 2021 these initiatives will be established, IP will be protected through patents.

3 Process innovation

New knowledge has been obtained on the application of CCU for the Chemelot site. The CCU white paper will strengthen our position related to CCS/CCU. Most likely we will perform a joint project with OCI and Sitech related to CCS.

4 Process safety and societal acceptance

The development of predictive modelling by use of AI and ML in WP4 for the purpose of enhancement of process safety, has raised awareness and interest from other companies at Chemelot (SABIC, DSM), the Safety Delta Nederland (SDN) as well as other companies inside and outside NL. The SDN has proposed to prepare cooperation with (a.o.) authorities, universities and VNCI in 2021. Other companies that have shown interest (some have requested for project proposals) are in the markets of recycling (GDF Suez Recycling), automotive (Nedcar), insurance (Germany) and oil and gas (ADNOC/Abu Dhabi and KNPC/Kuwait). In preparation of project proposals agreements (incl. protection of results wrt IP) will be prepared in NDA's.

5 Transition scenarios and system integration towards 2030-2050

The results of the project will help the industry to make well-founded decisions and develop robust and coherent transition pathways, taking into account uncertain developments in the outside world and making sure that all relevant stakeholders are involved. The results will help to better understand complex interactions (in markets, product chains, international economy, environment, innovation, circularity) on the longer term. We are approaching the Chemelot site users (including Sabic and OCI Nitrogen) to develop projects on sustainable product chains, the applicability of new technologies and availability of raw materials. We are planning to expand this by approaching companies in other industrial clusters soon.

Prospects for applications:

- 1. Shared innovation program Brightsite which will be the main marketing and business development channel to interact with market stakeholders, establish an overall innovation program and initiate spin-off projects
- 2. B2B projects will be developed on customer specific specialty applications related to the research topics due to increased market visibility and unique know-how and infrastructure developed at the field lab at the Brightlands Chemelot Campus and/or Chemelot site
- 3. Subsidized projects such as RVO and H2020 projects will be used to further enhance the knowledge position.

The currently involved Brightsite partners (Province of Limburg, Sitech Services BV, Brightlands Chemelot Campus and University Maastricht) have formulated their cooperation and the necessary provision of people, means and agreements on confidentiality in a Consortium agreement on June 25th 2019.

Publicity

1 Electrification

- M. Saric , Feasibility study Electric naphtha cracking,(TNO report)
- Y. Creyghton, Literature research report non-oxidative plasma conversion of methane (TNO report)

4 Safety & society

- Article. “HSE management in the era of Artificial Intelligence. A promising, predictive process safety model is under development.” Chemelot website. November 2020.
- Leaflet. “Vooraf voorspellen in plaats van achteraf verklaren. Een gamechanger binnen HSE-management”. November 2020.

5 Transition scenario’s

- “Cost-effectively reducing CO_2 emissions by saving on steam requires Chemelotwide approach”, Chemelot website, 9 november 2020.

Website: Brightsite Center | Transforming Industry Towards a Sustainable Future
https://brightsitecenter.com/

18 ERP Body-Brain Interactions

ERP Contacts: Jasper Kieboom (Project Lead), Jan van Erp, Robert Kleemann (Lead Scientist), Paulien Bongers (Science Director)
ERP Duration: 2020 – 2023

Progress 2020

Objectives

This ERP has two main objectives:

1. To develop a first body-brain platform for analysis of body-brain interactions in humans. This test facility will enable TNO
    a. to measure all sorts of body-brain interactions, i.e. biochemical metabolic, inflammatory, (neuro)physiological and socio-psychological parameters in conjunction with cognitive performance readouts;
    b. to develop predictive algorithms that employ the measured parameters to predict cognitive performance of a person.
2. To develop adjacent preclinical body-brain platforms that will complement human platforms and that will enable TNO
    a. to analysis tissues and identify causal mechanisms as well as molecular factors that signal between body and brain
    b. to test new treatments that could improve cognitive performance, attenuate brain inflammation and brain disorders, including dementias (critical for stakeholders and biomedical R&D).

To achieve these long-term objectives, a roadmap for the ERP has been developed (see graph) which was approved by the Science board of TNO. In the first year (2020) the ERP focused on human and mouse studies to identify key biological parameters (biochemical molecules, (neuro)physiological and psychological parameters) that determine cognitive performance and health.

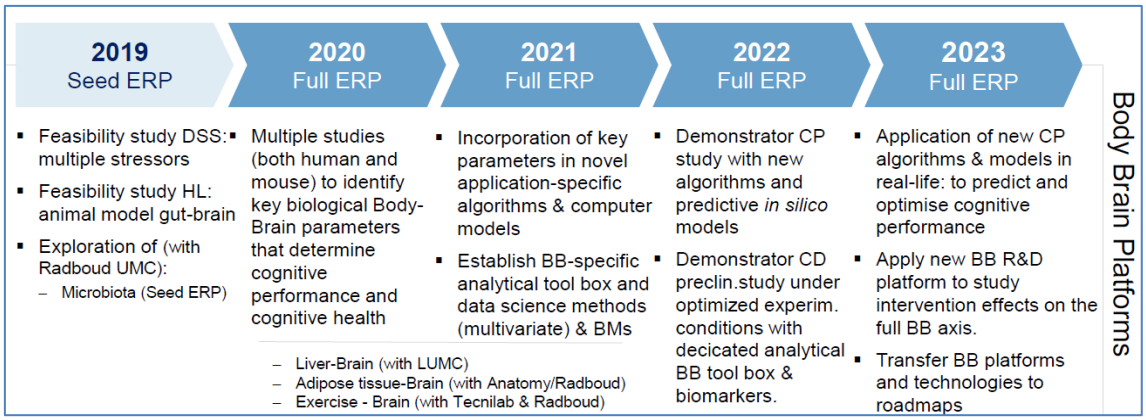


Figure 14: Full ERP body brains roadmap 2020-2023 | approach/results

The development of a body-brain platform for humans involves two types of studies: 1) a joint research clinical trial (with Radboudumc and Rijnstate hospitals; 'BARICO' trial) focusing on the more **chronic** metabolism and inflammation-derived factors that will determine cognitive performance; 2) an in-house human study which investigates how cognitive performance can be optimized under influence of **acute** stressors that perturbate metabolism or inflammatory state (exemplified by sleep deprivation as prototype acute stressors). The two types of studies are interlinked because acute stressors are superimposed on the chronic stressors that stem from metabolism and the inflammatory state. Information gained from 1) and 2) will enable us to identify body and brain-derived determinants of cognitive performance. Furthermore, the BARICO trial has broad relevance because it investigates the most common metabolic chronic stressor in humans, overweight/obesity, which is also critical for the government (e.g. Preventie Akkoord). The acute-stressor study has broad implications because the chosen prototype stressor, sleep deprivation, is the most common stressor in military and civil settings. Novel for both studies is that we characterize the *longitudinal dynamical* BB responses upon modulating

the stressors: In the case of obesity, participants will undergo metabolic (bariatric) surgery to lose weight with the aim to improve cognitive performance. In case of the acute stressor study, participants will be extensively phenotype prior to the sleep deprivation stressor regarding their dynamical response to e.g. social stress, visual or acoustic cues etc). These recordings will then be used to predict (via algorithms and correlations) the decline in cognitive performance after sleep deprivation. This enables us to identify body determinants that are critical for cognitive performance under chronic *and* acute body-brain stressors, and to identify shared common biological determinants that define the brain's cognitive performance, i.e. intersection of Research Lines (RL) 2 and 3.

In parallel, and with the objective to identify causal factors produced by specific organs (thus by the microbiota/gut, by the liver, or the adipose tissue in the state of obesity or by the muscle during exercise), mechanistic mouse studies will be conducted in a separate research line (RL1) allowing molecular studies of organs and demonstration of causality. The mechanistic studies described in the roadmap will lead to the development of a unique and comprehensive preclinical platform comprising all organs relevant for body-brain research for further use in roadmaps and at stakeholders (R&D studies).

The questions that will be addressed are:

1. Which body parameters (e.g. microbiota, plasma molecules, neuro-physiological parameters) are connected with which critical function of the brain (i.e. cognitive performance, memory capacity, cerebral blood flow, neuroinflammation) and how are they connected?
2. How can we use the measurable body-brain parameters to predict cognitive performance (or lapses in performance) of an individual using novel algorithms/models?
3. Is it possible to use the identified body-brain parameters and the new preclinical platforms to demonstrate that cognitive performance or brain health can be improved via the body-brain interactions identified in this ERP?

The main deliverables are thus novel and encompass complementary human and preclinical body-brain platforms, as well as the required enabling (analytical, data science) technologies to analyse their output (Body-Brain-analytics tool, Body-Brain-bioinformatics tools).

Within TNO, experts of the required disciplines are available at, among others, the units HL and DSS and will actively resolve the classical scientific segregation in beta and gamma disciplines. The ERP stimulates interaction between units and scientists to develop new tools and applications and open new market opportunities at cross-roads of established disciplines. An important objective of the ERP project is to provide an opportunity for talented medior/senior scientists and project leaders (e.g. from the Jong-Kennisberaad, or talent with potential in academia): they will receive responsibility as WP leaders to establish new connections between units that will, on the long-run, lead to innovate and strong technology position and new market perspectives at intersections between units.

Results realized

No.	Results planned	Realization
1	WP1.1 Established optimal experimental conditions for study of liver-brain interactions in preclinical platform	Yes
2	WP1.2 Establishment of optimal time-point for surgery in adipose tissue-brain study	Yes
3	WP1.2 Established optimal experimental conditions for study of adipose-brain interactions in preclinical platform	Yes
4	WP2.1 Safe storage of clinical trial samples (Barico)	Yes
5	WP2.2: Experimental design (including literature background) for the study on sleep deprivation as an acute stressor	Realized: Experimental design and its motivation was submitted to METC, and after revision, resubmitted and approved.
6	WP2.2: Start and first data of human intervention study	Partly realized in the form of the design and building set-up of an extra pilot/pre-study; data will be collected in 2020.
7	WP3.1 Develop method to enable analysis of transcriptome and lipidome from one small biopsy	Yes.
8	WP3.1 Establishment of a transcriptome. metabolome and/or lipidome dataset of Barico trial	Yes, transcriptome, lipidome & amino acid metabolome of all available 130 samples (from total 170) (Corona=delayed clinical trial;
9	WP3.1 Establishment of a micro- and mycobiome dataset from mucosal swaps	Moved to 2021 (Corona delay because of LAMP test development)
10	WP3.2 Evaluation of the use of analytical platforms to Barico samples	Yes

11	WP3.2 Pathway based biomarker selection for brain function	Yes
12	WP3.2 Association between biological parameters and cognitive performance	Yes
Additional	WP3.1. Establishment lipidome of circulating cells and erythrocytes (available BARICO samples)	Yes.
Additional	WP3.1. Cytokine profiling of available BARICO samples: baseline and surgery	Yes.
Additional	WP3.1. Liver lipid analysis of BARICO biopsies	Yes.
	Reports, papers, presentations planned	
1	WP4.3: Publication on data collected 2019 (Effects of noise and skipping a meal on cognitive performance and physiological markers of arousal and attention)	Bottenheft, C., Brouwer, A.-M., Stuldreher, I. V., Groen, E., & van Erp J.B.F. (2020) Cognitive task performance under (combined) conditions of a metabolic and sensory stressor: Cognition, Technology & Work.
2	WP4.3 Review paper on the interaction between homeostatic, motivational and control processes in obesity	Activity partly performed. The outcome was summarized in a ppt report and the involved scientists decided not to publish because of the too broad scope.
3	WP4.4: Review paper of various types of gut-brain interactions submitted to peer-reviewed journal	Activity stopped in Q1 2020 because of 3 comparable reviews that were already published.
4	WP4.3 Manuscript on the effects of the gut-derived metabolite propionate on body (metabolic health) and brain (cognition and brain functioning) in collaboration with RUMC	E. Gart, A. Tengeler et al., Propionic acid attenuates non-alcoholic steatohepatitis and improves cerebrovascular functions in obese Ldlr-/-.Leiden mice. FASEB J., 2020
5	WP1.1 Abstract on a new body-brain interaction for dissemination at scientific conference	Not submitted yet.
6	WP1.1 Presentation on potential causal role of liver-derived mediators that affect brain	Yes.
7	WP3.2: submitted scientific publication, in collaboration with Tilburg University, on acute and chronic (social) stressors on cognitive performance in adolescents	In progress, but probably not realized by the end of the year due to delays caused by Covid19 and personal circumstances of collaborators.
Additional	WP3.2: scientific publication on the relation between different biomarkers of vulnerability to stress, measured before the Covid-19 pandemic, and Covid-19-related emotional concerns.	In progress
Additional	WP3.2: published scientific paper, using data previously collected in the AMPERE project.	Van Beurden, M., Brouwer, A.-Met al. (2020). Towards user-adapted training paradigms: Physiological responses to physical threat during cognitive task performance: Multimedia Tools and Applications, 1-18.
Additional	(WP3.2): Scientific methodological paper on eye-tracking	In progress
Additional	WP1: scientific publication with Univ of Cambridge using the version 1.0 animal model of BBI (Ldlr.Leiden mice) in translation to children (infants) to predict development of obesity	Olga Laurentya, R.Kleemann et al., Lancet EBioMedicine, accepted (Dec 2020).
Additional	WP1: scientific publication with University of Sevilla in version 1.0 animal model of BBI on the effect of olive oil and polyphenols	Alvarez-Amor et al., Nature Scientific Report, in revision
Additional	Establishment of collaboration with University of Munich; Institute for Stroke and Dementia Research. ERP provided samples of the v1.0 BBI Ldlr-/- mouse model.	Acknowledged in Kontos et al., Nature Communication, 2020.
Additional	Writing of an NWO proposal for a grant on neurobiology and the development of dementias using a combined human patient and mouse approach for mechanistic insight. Collaboration with Neurology of Radboudumc.	First round passed; rebuttal has been submitted Dec 2020.

Realized contribution to new knowledge and technology

In the first year of the ERP project, we set significant steps towards the two main technological goals: development of a human body-brain (BB) platform and a complementary preclinical BB platform. More specifically, new technologies and experimental setups for a first human BB test facility were established and validated in dedicated studies with volunteers. In parallel, a first prototype preclinical BB test model v1.0 was established: the Ldlr-/-.Leiden mouse on specific human-like diet. The human and animal BB platforms are complementary and we have developed new biological and bioinformatical techniques to couple them. For instance, we have invested in metabolomics and lipidomics analyses that can be employed in humans and animals allowing direct 1:1 comparison and translation. We also invested in gene expression profiling on the level of pathways and upstream signaling receptors and master regulators of inflammation and metabolism that can be used in human studies and in experimental models. For instance, we used human-derived gene expression signatures that characterize particular immune cells and employed them in the BARICO dataset to get a first quantitative readout of how many immune cells are present in the human livers. In parallel, this technique has been adopted and used in the roadmap BMH to estimate the number of mouse immune cells in liver (published in vd Hoek and Kleemann et al., Cells, 2020). The ERP also has developed a new way of sampling small aliquots of human blood (using preclinical technology from mice) and these small aliquots of blood will enable us to profile and characterize human volunteers in the human BB platform on molecular level including amino acid profiling, lipidomics and cell membrane analyses as well as cytokine profiling, all performed in 3 droplets of human blood using ERP technology. A cornerstone of the biological technological advances for the human studies is the rather unorthodox use of tissue sampling and processing tools from mice. The mouse toolbox is intrinsic to the size of these animals optimally equipped to outperform the conventional human research tools which rely on large quantities of blood and tissue. In the ERP, completely converted the mouse toolbox to humans allowing novel biochemical measurements of gene expression, lipid composition, metabolism (amino acids etc.) in order to characterize human volunteers that perform cognition tests or that are exposed to (different kinds of) stressors. Because of these new tools and the possibilities to understand the interaction between cognition (brain) and the body, the METC protocol for an ERP study was very smoothly accepted (Dec 2020) and we now set out to identify the physiological and organ-derived parameters that are responsible for cognitive performance and the usually experienced decline in cognitive performance after deprivation of sleep. In sum, we will gain understanding of the connecting mechanisms between body (see approach on graph right) and this insight will enable us to delineate new avenues for rationale-based intervention utilizing either psycho-social strategies alone or in combination with molecular pharmaceutical or nutritional strategies.

On a national strategic level, the ERP is fully in line with the strategy of governmental departments and (inter)national TNO stakeholders, among which nutrition, pharmaceutical and diagnostic industries. The specific departments and roadmaps are illustrated in the graph below.

Figure 15:Coherence of ERP strategy with National roadmaps.

The interest from stakeholders in our project is supported by the fact that we succeeded in establishing many collaborations with external partners and that we will launch a parallel PPS to this ERP called GLoBAL (Gut-Liver-Brain-Axis-Links in obesity). Overall the stakeholders' interest is twofold:

1) It became clear that most stakeholders are interested in the biology component of the body-brain axis and potential new strategies to optimize cognitive performance via modulation of biological mechanisms, thus via routes of metabolism and via modulation of the molecular interplay between organs that signal to brain or that supply the brain with nutritional components required for optimal brain functioning.

2) The main technology products are BB testing facilities or test models allowing to i) characterize an individual regarding his/her body-brain interactions; ii) predict his/her cognitive performance under conditions of acute or chronic stress; iii) test new interventions targeting the body that can improve cognitive performance and brain health.

External Collaborations and PhDs: The ERP improved TNO's technology and knowledge position on BB interactions significantly because we were able to team up with key players in the field of body-brain research and preclinical (test) models thereof (e.g. University of Munich-Institute for Stroke and Dementia Research, Donders Institute Nijmegen, Radboud Medical Center, Leiden University Medical Center, Tilburg University, Ghent University). With the department of Anatomy (Radboud), we obtained a ZonMw grant for neuroimaging studies on muscle-to-brain interactions in mice. With the department of Neurology (Radboud), we are now in the second round of a large ZonMw Open Competition Consortium Call). The number of publications and PhD students that participate in this ERP is exceptional. There are 2 PhD students working on the human BB platforms specifically (Bottenheft & Stuldreher); one PhD student that combines BARICO with preclinical work (Seidel); one PhD student for the BARICO trial (Vreeken); two PhD students that concentrate on gut-brain (Tengeler) and muscle-brain (Lohkamp) interactions in the preclinical model systems.

Realized contribution to the market position

So far, the ERP demonstrated that the main interest of TNO stakeholders, when market criteria and tools/technologies for subsequent exploitation are concerned, is related to modulation of the psychological component and the biology component of the body-brain axis. With respect to brain, the interest of TNO stakeholders is twofold: a part of the stakeholders (e.g. defense) is primarily interested in optimization of cognitive performance under acute and chronic stressors (preferably combinations of both) and prediction of cognitive performance under challenging situations, for instance to become more alert when upcoming lapses of attention are predicted.

A second group of stakeholders is interested in the biomarkers and the molecules that signal between body and brain as they could provide tools to monitor health or to signal upcoming disorders of body and brain. With the biomarker company Nordic Biosciences and the Maag Lever Darm Stichting we have now agreed to launch a PPS (GLoBAL-1) in Q1-2021 to investigate new sorts of biomarkers developed on tissues obtained from our research, and to unravel the interrelationship between gut processes and consequences in liver or brain.

In addition to this, a third group of stakeholders (mainly nutritional and pharmaceutical companies) are interested in the health applications of body-brain research: for instance, nutritional or pharmaceutical strategies to prevent the development of cognitive impairment or improvement of vascular/brain inflammation. We have close contact with a company who would like to use the v1.0 preclinical model for investigating the potency of holistic medicinal concepts that affect organ health and thus also the brain and the cognitive functions. This company has requested budget to participate in the aforementioned PPS which will be set up adjacent to the ERP. Other nutritional companies with interest in our concepts and the autoregulatory capacity of the human body are Japanese and Norwegian food and nutrition companies, as well as pharmaceutical industries in the US.

The commercialization routes of body brain research are thus manifold and it should be noted that the psycho-social aspects which are very critical for implementation of any strategy are, by themselves, difficult to commercialize. Based on the results of the ERP so far, and the input generated from the various groups involved, the market potential was considered greatest if the ERP would focus on 'the biological axis affecting cognitive performance'. The initial broader focus and aim of the ERP (to integrate beta and gamma sciences approaches) was considered too vague regarding 'end deliverables' and ambiguous ('rather a tool than a product') regarding the path towards the anticipated deliverables over a 4-5 years period.

Publicity

Publications

- Vreeken et al.., Study rationale and protocol of the BARICO study: a longitudinal, prospective, observational study to evaluate the effects of weight loss on brain function after bariatric surgery. British Medical Journal Open 2019.
- Gart et al. Propionic acid, and not Caproic acid, attenuates non-alcoholic steatohepatitis and improves (cerebro)vascular functions in obese Ldlr-/-.Leiden mice. FASEB Journal., 2020
- Alvarez-Amor et al., Extra virgin olive oil improved body weight and insulin 1 sensitivity in high fat diet-induced obese LDLr-/-.Leiden mice 2 without steatohepatitis attenuation. Nature Scientific Reports, 2020, in revision.
- Bottenheft, C., Brouwer, A.-M., Stuldreher, I. V., Groen, E., & van Erp J.B.F. (2020) Cognitive task performance under (combined) conditions of a metabolic and sensory stressor (link: https://link.springer.com/article/10.1007/s10111-020-00653-w) Cognition, Technology & Work.

- Van Beurden, M., Brouwer, A.-M., van Baardewijk, J.U., Binsch, O., Vermetten, E., & Roijendijk, L. (2020). Towards user-adapted training paradigms: Physiological responses to physical threat during cognitive task performance (link) Multimedia Tools and Applications, 1-18.

Conferences

- Bottenheft et al., 2019. Understanding the effect of mental and physiological stressors on cognitive performance. Poster presentation at the 3rd International Symposium on Human Mental Workload: Models and Applications (H-WORKLOAD 2019) in Rome
- Gart et al., 2019. Propionic acid intervention in obese Ldlr-/-.Leiden mice attenuates NASH development, but negatively affects cognition. Poster presentation at the EASL NAFLD summit 2019 (Seville, Spain). This poster was awarded 'Best of NAFLD Summit'.
- Gart et al., 2019. Propionic acid intervention in obese Ldlr-/-.Leiden mice attenuates NASH development, but negatively affects cognition. Poster presentation at the 13th European Nutrition Conference, FENS 2019 (Dublin, Ireland).

Patents, technology references.

Preclinical BBI model used and referred to in:

- Laurentya and Kleemann et al., Lipid ratios representing SCD1, FADS1, and FADS2 activities as candidate biomarkers of early growth and adiposity. Lancet- EBioMedicine 2020, conditionally accepted.

Kontos et al., Designed CXCR4 mimic acts as a soluble chemokine receptor that blocks atherogenic inflammation by agonist-specific targeting. Nature Communications 2020.

19 ERP Social XR

ERP Contacts: Maria Boen (Project Lead), Omar Niamut (Lead Scientist), Paul Havinga (Science Director)
ERP Duration: 2020 – 2023

Progress 2020

Objectives

In the ERP Social eXtended Reality (XR) we aim to create a shared XR environment, where participants get the feeling of being in the presence of, and interacting with, other persons at a remote location. Social XR will provide the full spectrum of presence: telepresence (the extent to which one feels present in the mediated spatial environment), self-presence or body ownership (the extent to which the virtual self is experienced as the actual self), and social presence or co-presence (the sense of being in the company of other persons). The addition of haptic interaction will provide both the experience that one is physically present in the mediated environment, and enhance the mediated representation of the remote partner. With the ERP Social XR, TNO aims to become an international leader in the field of photorealistic representation and communication between multiple people in networked virtual environments. TNO is building its technology base from 5G, social VR, and haptic interactions into an integrated and fully-fledged facility for sharing AR/VR experiences across different locations and through sensory modalities beyond sound and vision. TNO can distinguish itself in this way from knowledge and market parties that mainly use AR/VR to create individual, location-based experiences and applications, in which communication and other forms of interaction between people at remote locations hardly play a role.

In this ERP, the objectives are as follows:

1. To develop and validate core technology for shared and social networked XR experiences, that i) allows for 6DoF human representation through volumetric media, ii) integrated with social touch features through tactile/haptic interaction systems, and iii) can be deployed on a distributed softwarized mobile networking infrastructure.
2. To demonstrate and validate the application potential of the technology being developed; aligned with unit roadmaps, and in later stages, based on stakeholder interest.
3. To set up collaborations with key partners and stakeholders, by interacting with the outside world and by demonstrating both components and integrated PoCs at key academic and industry events;
4. To strengthen the knowledge and technology positions of the Research Groups involved.

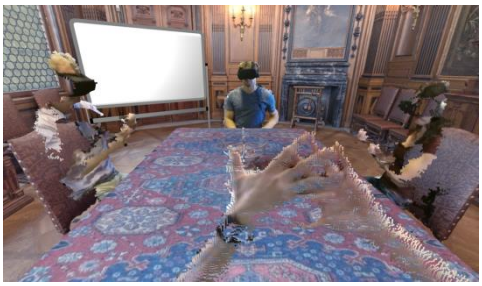


Figure 16: Example of shared XR environment, developed in 2019 as part of Seed ERP Social XR

Results realized

Project 1: Immersive Experiences

No.	Results planned	Realization
	Project 1: Immersive Experiences	
1-1	Proof-of-principle of the orchestrated automated calibration and synchronization of a networked multi-camera configuration. Demonstrate using improved eye-contact	Yes
1-2	Proof-of-principle and conference publication of an efficient hybrid video and point cloud data coding and streaming format. Demonstrate using 3D hand position with self-view	NO, is postponed
1-3	First design of tactile data streaming format → A Tactile Proxy between VR environment and Tactile displays that supports different types of tactile displays with their own modality is build.	Yes

1-4	Minimal set of measures and conference publication that maximally describes the quality of the mediated social communication experienced at different affective (sensory, perceptual, and decision making) processing levels	Yes (EuroVR2020, Holistic Quality Assessment of Mediated Immersive Multisensory Social Communication)
1-5	Initial guidelines on the synchronization (in-)tolerance of visual, auditory, and haptic social cues	Partially, will be elaborated in 2021

Project 2: Empowered Edge

No.	Results planned	Realization
2-1	Proof-of-principle of the instantaneous, automated and orchestrated deployment of Social-XR processing modules on the edge and cloud infrastructures; version 1 has focus on orchestration and GPU virtualization, version 2 has is based on monitoring and includes flexible processing (e.g., mobility)	Yes
2-2	Report and conference publication about edge computing placement and flexible media processing	Yes (MMSys 2021, Assessing Latency vs Quality Trade-offs of Moving Processing for Photo-realistic VR Conferencing to the Network Edge)
2-3	First design and integration of edge computing infrastructure in TNO's Hi5 platform, with high-bandwidth (>100 Mbits) and low-latency (< 5ms) access to edge computing resources	Partially, will be elaborated in 2021
2-4	First design and integration of real-time network and infrastructure monitoring	Partially, will be elaborated in 2021
2-5	Report and conference publication on the performance of 5G radio access networks in different simulation scenarios that captures the characteristics of mmWave radio channels and provides solutions at link/network layer to deal with the intermittent nature of these channels, in the context of Social XR applications	Yes (2021 Joint EuCNC & 6G Summit, Performance Modelling for Social VR Conference Applications in Beyond-5G Networks)
2-6	Test setup that allows for experimentation with different 5G mobile networking scenarios	Yes

Project 3: Showcases

No.	Results planned	Realization
3-1	Report on requirements for a set of showcases, based on specific interests from several TNO units	Yes
3-2	Set of mockup demonstrators, based on the showcases derived from specific interests from several TNO units	Yes
3-3	Report on the evaluation of this set of mockup demonstrators	Yes

Realized contribution to new knowledge and technology

In 2020, within the ERP we have focused our research on three main tracks:

Track I: Immersive Experiences

State-of-the-art: In our digital age, human social interaction is often mediated. Current systems like Skype and FaceTime stream vision and sound, but do not yet include other sensory modalities. To enable affective human communication and bonding, future generations hardware and software should be able to provide full, multisensory communication and experience. As a first step toward full multisensory reality, we start with adding touch to a video-based social VR experience, because touch is our primary non-verbal communication channel for conveying intimate emotions and as such essential for our physical and emotional well-being. However, even though there is increasing evidence that mediated touch affords affective human communication and bonding, current communication systems (such as videoconferencing) still do not support communication through the sense of touch. As a result, mediated communication does not provide the intense affective experience of co-located ("shared space") communication. Sharing a VR space with multiple participants or devices is already feasible in location-based systems, where local connectivity is provided through a fixed or Wi-Fi network. Networked social VR experiences are available through most of the major VR platforms, but mostly consider avatar-based participant representations, e.g. Facebook Horizon[5]. Volumetric capture of humans mostly

[5] https://www.oculus.com/facebook-horizon/ Facebook Horizon, VR is better with friends

requires expensive capture systems (e.g. Vologrames[6] and Volucap[7]) and social and collaborative VR applications in which participants are captured with low-cost commercially available (depth) cameras are still rare; Mimesys[8] is the primary example. Within the H2020 VR-Together project[9], TNO has developed TogetherVR, a web-based networked platform for social and collaborative VR experiences.

Desired situation: the research and development activities in this track should enable us to determine a significant and valuable niche in the area of volumetric video for shared and collaborative XR experiences. These include a real-time acquisition system for performing a volumetric scan of all participants, e.g. how to store and synchronize the data; insights into the trade-offs between using 2D video-based and native 3D representations of volumetric video, e.g. what is the optimal trade-off between resolution and latency; and a draft architecture for an end-to-end transmission and rendering pipeline for volumetric video. In addition, tactile sensors and haptic devices will record people movements and send feedback to people.

Research topics: We investigate **multi-camera configurations** that capture color and depth information from the participants in a social XR experience. Such capture systems are typically construed by arranging depth sensors in an inward-facing configuration. They require automated calibration and synchronization of resulting captured data, such that point cloud data can be generated and rendered at runtime, aligned on a 3D geometrical plane. By improving the current technology in terms of calibration and synchronization, we will establish true volumetric video capture. With respect to **coding and streaming**, we study both (hybrids of) video based as well as 3D geometry orientated coding methods and associated container formats, to select the most efficient and robust volumetric video and tactile data representations for transmission over mobile networks, under latency and bandwidth constraints. In particular, we investigate suitable protocols for real-time and efficient **delivery of tactile data**. For rendering of volumetric video, we aim to develop new shaders that can cope both with multiple incoming color-plus-depth data streams, and with the mapping of 3D hand positions in relation to the position of the user. To provide an immersive experience comparable to face-to-face communication, our envisioned system should reliably convey information about both the shared environment (VE) and about all relevant **social cues**. Important issues are (1) the **synchronicity** between the different sensory signals that is required to achieve a coherent multisensory experience and (2) the **bandwidth** required to optimally convey relevant social cues (e.g., gaze direction, eye contact, prosody, facial expression, non-verbal sounds, gestures, body posture, orientation and proximity, social touch, collaborative haptics, pupil size, eye blinks, etc.). The coding of volumetric video and tactile data should be sufficiently efficient, and typical internet networking effects such as time delays, jitter, or packet loss should be minimized to maintain the levels of system transparency and stability that are required to provide an ***immersive and synchronous multisensory communication experience***.

Contribution to the acquaintance of new knowledge and technology: i) a proof-of-principle of the orchestrated automated calibration and synchronization of a networked multi-camera configuration; ii) a proof-of-principle of an efficient hybrid video and point cloud data coding and streaming format ; iii) a first design of tactile data streaming format; iv) a demonstration of improved mapping of 3D hand positions relative to the user; v) a demonstration of improved eye contact; vi) a minimal set of measures that maximally describes the quality of the mediated social communication experienced at different affective (sensory, perceptual, and decision making) processing levels; vii) initial guidelines on the synchronization (in-)tolerance of visual, auditory, and haptic social cues, and viii) a report on how to deal with typical internet networking effects and on how to determine a good benchmark regarding these challenges.

Track II: Empowered Edge

State-of-the-art: Emerging 5G network technology, powerfully integrating data transport, storage and computing, has the potential to enable new, innovative and highly demanding applications, such as shared and collaborative AR/VR. It promises ultra-high bandwidths at the radio access and ultra-low end-to-end latencies. Moreover, through a high degree of ‘softwarization’ 5G networks are extremely flexible and allow the creation of virtual networks (“network slices”) on top of the underlying infrastructure that can be tailored to specific applications. Although network slicing has been addressed quite extensively by the research community at the conceptual level, the actual configuration and management of network slices (and the involved resources) to meet the requirements of the applications under realistic, highly dynamic network usage conditions is still an open research area. Focusing on the radio access network, another major research challenge is how to deal with the intermittent nature of ultra-high frequency wireless channels needed to achieve the high throughputs required for VR-based applications Moreover, for VR-based applications the tight latency requirements should also be taken care of, besides the need for stable high throughputs.

[6] https://vologrames.com/ Vologrames, Bring real people to immersive media.
[7] http://www.volucap.de/ Volucap, the volumetric capture studio
[8] http://www.mimesysvr.com/ Mimesys, the first holographic meeting platform
[9] http://vrtogether.eu/ VR-Together, the feeling of being there together and the photorealistic quality of the content

Desired situation: We aim for new insights into network resource orchestration, e.g. which data of which quality do we need where in the processing and transmission chain, for new volumetric video and tactile data. A high degree of automation will be required to run the powerful, though, complex 5G systems. In particular, we envision seamless orchestration and reconfiguration (e.g., scaling up) of network slice resources in run-time, on demand of the applications (cross-layer optimization) as well as based on continuous system monitoring, and supported by Artificial Intelligence. Humans will remain in the loop, but according to an intent-based model, i.e. for more and more tasks people only have to state “what” they want to have rather than “how it should be achieved”.

Research topics: To be able to leverage the full potential of edge computing, (1) edge computing has to be tightly integrated into the 5G infrastructure and instantiation of resources on the edge nodes and in the cloud has to be **orchestrated** such that resources are made timely available to the Social-XR clients; (2) edge resources have to be discovered by the clients and network connections between the clients and the edge nodes, and between the edge nodes and a central cloud, have to be **configured** and established; and (3) the Social-XR clients and infrastructure have to be configured for optimal use of the available **computing and transmission resources**; (4) continuous **monitoring** of the Social-XR service needs to be in place and the mechanism for the correcting actions (e.g., re-allocation or resizing of the components) need to be available supporting dynamic and flexible processing of the media streams. We will study these aspects, starting with the **integration, localization and deployment** of edge computing resources, focusing on the high-bandwidth and low-latency connectivity to the edge computing resources, along with the associated benefits and the costs. Important factors for the performance of the Social-XR service are the capabilities of the edge node (e.g., CPU, RAM, and GPU availability) and the network performance (e.g., throughput, latency, and jitter). As such, we will enable **GPU acceleration and virtualization** in our computing infrastructure and we will develop an **orchestrator service** based on TNO Research Cloud/Hi5 platform that automatically and dynamically deploys, re-deploys, scales in and out modules of the Social-XR service at various places in the network (i.e., on both edge devices and centralized servers, depending on the configured policies and telemetry), making the Social-XR modules available as application functions in the mobile network. With respect to optimally using the edge infrastructure and network resources, we will study which **key performance indicators** have to be extracted from the edge computing infrastructure and 5G mobile network, in order to serve as input parameters for a dynamic orchestration and configuration platform.

As part of this application and infrastructure/network integration, it is important to understand the network connectivity to the edge, including the characteristics of 5G radio access networks (RANs). We will study how RAN performance translates to the application layer performance, such that the application can properly adapt to the situation and the network can provide QoS when this is needed. Based on existing work and network simulation techniques, we will investigate the vulnerability of mmWave channels for blocking and its effects on throughput, throughput variations, latency, jitter, and packet loss. We will use these results to build a test setup that allows for experimentation with the Social-XR application under different networking conditions. The test setup will make use of a network emulator developed by TNO. Finally, the information about various parameters of the (emulated) RAN will also serve as input data to the metering system, which in turn makes the performance parameters available to the Social-XR application.

Contribution to the acquaintance of new knowledge and technology: i) a proof-of-principle of the automated, orchestrated and monitored deployment of Social-XR processing modules on the cloud and edge infrastructures; ii) an integration of a network and infrastructure monitoring service iii) a report and conference publication about edge computing resource placement, indicating the (potential) benefits of edge computing integration; iv) a report and conference publication on the performance of 5G radio access networks in different simulation scenarios that captures the characteristics of mmWave radio channels and provides solutions at link/network layer to deal with the intermittent nature of these channels, in the context of Social XR applications; the conference publication focuses on the link/network layer solutions; v) a test setup that allows for experimentation with different 5G mobile networking scenarios.

Track III: Showcases

State-of-the-art: XR has the potential to impact our lives [12]. Social presence has been studied extensively in the past. Human factors research on telepresence, social connection and social touch is available.

Desired situation: Several TNO Units (specifically; DSS, HL, ICT, TT) are interested in holographic communication and its constituent technologies. With such a system, national security personnel (e.g. police officers) can ask for remote assistance and discuss with expert colleagues about crime scenes on location; distributed teams of soldiers can jointly train for critical missions; companies can let personnel meet and discuss remotely, and public services offering new mobility concepts can add an new modalities to their portfolio. Application of social XR technology should support the (professional) end user in his/her work, i.e., add aspects to working in teams at a distance that improve the performance, social presence and -interaction, or learning of the end user.

Research topics: To make sure that social XR technology actually supports the end user in working together at a distance in a way that improves on relevant aspects of his/her task execution, several relevant requirements can be identified: (1) the chosen applications need to fulfil a need of the end user, i.e. should be relevant, practical, and ideally solving a problem, (2) the technology should be intuitive to use, not adding additional challenges to the task/interaction, and (3) social XR technology needs to be evaluated in the applied context. The requirements form the basis for two main research questions in Track III; i) how can the relevant social XR technology be applied in the different domains of the TNO Units? And ii) does the envisioned social XR technology improve social presence in the applied contexts, and if yes, how? For this second question, we aim to study the relation between and importance of telepresence and social presence with respect to the envisioned social XR technology, and explore up to what extent social XR can satisfy human needs for communication from mobility and sociological perspectives.

Contribution to the acquaintance of new knowledge and technology: The goal of the mock-ups is to show the potential of the technology and to evaluate research questions to develop new knowledge. It is not foreseen to integrate 'new' technology of the other work packages, but to use existing technology. The evaluations will lead to new insights regarding possible scenarios, regarding (technical) requirements as input for the following years of the ERP for further research and development of our social XR platform, and new knowledge on (human factors) research questions.

Social XR is also linked to **MoD research** programs, such as "Human Factors in Immersive Technology" (NL: 'Immersie op Maat'). These projects mutually benefit from transfer of knowledge and R&D equipment. The program is linked to the goals of the **topsector HTSM**, roadmap ICT. Specially, as part of the new Kennis- en Innovatie Agenda Sleuteltechnologieën 2020-2023, the Meerjarenprogramma on **Beyond 5G** Future Networks and Services includes holographic communication as one of the primary application challenges. Furthermore, the Dutch ministry of Economic and Climate Affairs has taken a specific interest in VR, as expressed in the "*Kamerbrief met reactie op het rapport Verantwoord virtueel; bescherm consumenten in virtual reality"* (December 3, 2020).

Realized contribution to the market position

Remote volumetric telepresence and collaboration is poised to be the killer app of augmented and virtual reality. Applications include gaming, attending live events, consuming content, shopping, dating, education and training, conferencing and more. In 2020, we have identified two main use case classes where we can create unique propositions. In the short term, we expect to provide value to XR meetings, e.g. business and family meetings. In the longer term, we expect to provide value to expertise-at-a-distance scenarios, for e.g. tele-education and training, and remote maintenance and support.

We have strong internal and external connections with roadmaps, programs and R&D agendas. In 2020, we have established specific links with the following Unit roadmaps, VPs and associated PMCs:

- PMCs Immersive Human Communications and Customized Digital Infrastructures from PMC cluster Fast and Open Infrastructures, as part of ICT roadmap and VP ICT in Unit ICT;
- PMC cluster Simulation, Education & Training as part of Operations & Human Factors roadmap in Unit DSS;
- Smart and Sustainable Mobility roadmaps of Unit T&T (e.g. not to travel);
- National Safety roadmap (e.g. remote assistance by police) in Unit DSS;
- Digital Health Technology roadmap (e.g. PMC4-Health apps) for Unit Healthy Living.

In the ICT roadmap, the PMC cluster Fast and Open Infrastructures includes the PMC Immersive Human Communication. This PMC is currently based on a 2D video-based social VR platform, with a 1-3 year market take-up expectation. This ERP will feed into an evolution of this PMC, for market take-up in 4-7 years. At Unit DSS, this ERP can contribute to roadmaps Operations and Human Factors, where XR technologies are used to support military personnel in their mission preparation and robot operation; and National Security, where XR technologies are used for training purposes and immersive robotic operation.

Furthermore, KPN is currently a stakeholder and partner in TNO VR knowledge base at Unit ICT. Several past and current projects in the KPN long-term research program focus on generating and standardizing IP for coding, streaming and orchestration technologies. Results from this ERP will therefore presumably be jointly protected with strategic IP partner KPN through the KPN long-term research program, unless determined otherwise.

Publicity

Papers

- Leonor Fermoselle, Simon Gunkel, Frank ter ter Haar, Sylvie Dijkstra-Soudarissanane, Alexander Toet, Omar Niamut, and Nanda van van der Stap., *Let's Get in Touch! Adding Haptics to Social VR*. conference paper for the ACM International Conference on Interactive Media Experiences (IMX '20), 17-19 June 2020Alexander Toet, Tina Mioch, Simon Gunkel, Camille Sallaberry , Jan B.F. van Erp and Omar Niamut, Holistic Quality Assessment of Mediated Immersive Multisensory Social Communication, conference Demo paper for the EuroVR 2020 Conference (won Best Demo paper Award)
- João Morais, Sjors Braam, Remco Litjens, Hans van den Berg., *Performance Modelling for Social VR Conference Applications in Beyond-5G Networks,* conference paper for 2021 Joint EuCNC & 6G Summit, 8-11 June 2021
- Lucia D'Acunto, Rick Hindriks, *Assessing Latency vs Quality Trade-offs of Moving Processing for Photo-realistic VR Conferencing to the Network Edge*, conference paper for NOSSDAV workshop co-located with the MMSys conference in 2021
- Toet, A., Heijn, F., Brouwer, A. M., Mioch, T., & Van Erp, J. B. (2020). An Immersive Self-Report Tool for the Affective Appraisal of 360º VR Videos. *Frontiers in Virtual Re*ality, 1, 14

Reports

- Sylvie Dijkstra-Soudarissanane, Frank ter ter Haar, Leonor Fermoselle Silva Pereira, Alexandre Silva Pratas Gabriel, Martijn van den Heuvel, Potetsianakis, Emmanouil, Simon Gunkel, Alexander Toet, Omar Niamut *ERP SXR - Project 1: Immersive Experiences*, TNO Report
- Lucia D'Acunto, Hans van den Berg *ERP SXR - Project 2: Empowered Edge*, TNO Report
- T. Mioch, A. Toet, S. Ganesan, H. Stokking, E. Abels, K. El-Assal, T. Klunder, *ERP SXR - Project 3: Showcases*, TNO Report
- Sylvie Dijkstra-Soudarissanane, *TNO and Meander: Collaboration towards XR Communication for elderly at care homes*, Draft TNO Report

Presence/events

- Prominent online presence in upcoming Smart Society Campaign

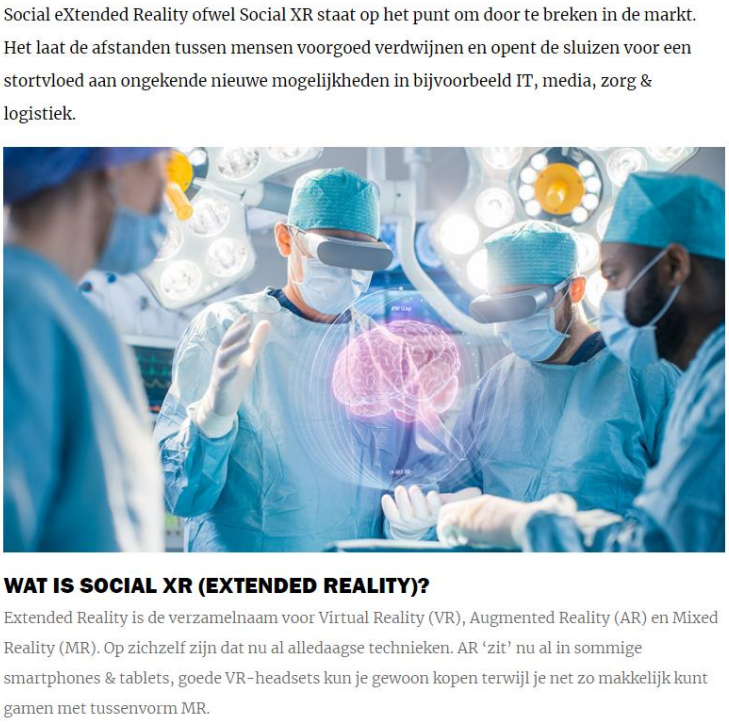


Figure 17:Newsitem on Smart Society Campaign
https://www.tno.nl/nl/aandachtsgebieden/informatie-communicatie-technologie/roadmaps/fast-open-infrastructures/social-xr-extended-reality/

- Presence at VR Days:

"Last week, colleagues Klunder, T.E. (Tessa), Rahim, M.G. (Galit) and Veen, T. (Teun) van der represented TNO at the VR Days Europe 2020. AT TNO's virtual booth, attendees could hear about our developments on volumetric video and haptics, through videos with Haar, F.B. (Frank) ter, Fermoselle Silva Pereira, L.I. (Leonor) and Heuvel, M.J.R. (Martijn) van den. At the booth of H2020 project VR-Together, Gunkel, S.N.B. (Simon) and Koninck, T.J.I. (Tom) de represented TNO. Attendees could hear about the world's first volumetric video conference over a public 5g network, realized by our partner CWI and KPN."

Figure 18: TNO's presence at VR Days

Online videos

- Video on collaboration with Meander, "Combat loneliness with Social XR": https://www.youtube.com/watch?v=ZNQK97d6ZB8
- Video on the potential of social XR to bring people closer together: "Met kerst dichter bij dan ooit dankzij XR-technologie" https://www.youtube.com/watch?v=lnaL6vGNyI0

20 SEED ERP Climate and Air Quality

ERP Contacts: Rianne Dröge (Project Lead), Martijn Schaap (Lead Scientist), Ardi Dortmans (Science Director)

ERP Duration: 2020 → Promoted to Full ERP

Progress 2020

Objectives

The overall goal of the ERP 'Climate and Air Quality' is the development of a globally applicable, multi-scale atmospheric modelling system with resolution down to 25m to fully exploit the emerging observation capacity from satellites and sensors. In addition to the work packages devoted to develop and advance methodologies that enable to perform realistic simulations at this unprecedented resolution, a system integration approach is taken to ensure that a complete and flexible modelling system is obtained. The new system will be demonstrated for the greater Eindhoven area, motivated by the secured access to (sensor) data, commitment of local policy makers, collaboration with ERP 'ExpoSense' and the presence of diverse emissions from transport modes, agriculture and households. The updated formulation provided above is a result of the seed-ERP progress made this year.

The aim of the Seed-ERP was to create a full-ERP proposal. The formulation of this proposal was based on the following components:

- System design document: describing the functional and practical design of the modelling system, including a list of models and data sources and a flow diagram showing how they will be integrated.
- Review document: describing findings from literature review and expert consultations.
- Demonstrator: demonstrating the feasibility of the envisaged modelling system and its added value compared to currently available systems.
- Business plan: describing the potential to exploit the model system, including potential customers and their research needs.

The different components are described in more detail in the plan of work for 2021.

Background and motivation

Every year around 7 million people die prematurely from exposure to polluted air. Global warming may lead to catastrophic sea level rise, droughts, and increases of wildfires and tropical storms. Critical loads for atmospheric nitrogen deposition are exceeded in 72% of the Dutch nature areas (55% in Europe), leading to significant biodiversity loss. All these pressing environmental challenges relate to anthropogenic emissions into the atmosphere and their negative impact on the environment. To curb these impacts, the Dutch government has committed itself to reduce the adverse health impacts due to Dutch emissions by 30% and to reduce greenhouse gas emissions by 49% in 2030, while nitrogen policies are currently under fierce societal debate. Many stakeholders have developed their own targets, e.g. climate neutral cities. These reduction targets will impact all economic sectors in the Netherlands, but the challenge is to decide which mitigation strategy to follow. Therefore, a strong demand exists for high quality and high-resolution information on the state of the environment, the origin of the pollution and independent monitoring of the effectiveness of implemented or planned mitigation options. The high-resolution is required for emission monitoring on local instead of national level and determination of more specific source-effect relations.

Two of the main challenges for providing such information are the need for high-resolution time-dependent emissions and the fact that the emissions and their impact are separated in time and place, influenced by complex processes such as atmospheric mixing and chemistry. At present, distinctly different model systems are used to describe these complex processes, each targeting specific spatial (urban to global) and temporal scales. However, there is a strong interaction between the different scales that needs to be considered when addressing above-mentioned environmental challenges. The main challenge, both conceptual and technical, is then to combine complementary models in one framework and to get those models to exchange information in a consistent and efficient manner.

Right now, the increasing resolution and quality of satellite and sensor data and the tremendously growing information on emitting activities through internet of things (e.g. real time traffic data) provides a driving force allowing a fundamentally different approach to detail the emissions and their environmental impact. To interpret these observations and provide high quality atmospheric information about the state of the environment and the impact of mitigation options to stakeholders, several fundamental challenges need to be resolved, which will be addressed in the full ERP (starting in 2021).

Results realized

No.	Results planned	Realization
1	Use case description	Yes
2	Functional and practical design of the modelling system	Yes
3	Emission maps for the demonstrator for agri-CH4 and traffic-NO_x	Yes
4	Collaboration agreements with TU-Delft and Wageningen University (WUR) on LES modelling (within Ruisdael), TU-Delft on data assimilation, and MPI for Biogeochemistry for CO_2 exchange modelling	
5	Business plan	Yes
6	Modelled distribution of NO_x, CH_4 for LOTOS-EUROS, US and DALES	Yes, although idealized case studies for DALES were performed
	Reports, papers, presentations planned	
1	Review report	Yes
2	System design document	Yes
3	ERP-proposal	Yes
4	2-3 presentations at conferences (EGU, AGU) or workshops	2 (online) presentations (ICOS Science conference & Freiburger workshop)
5	Submission of publication on the added value of the high-res calculations over Eindhoven in comparison to 2x2 Km LOTOS-EUROS runs and annual urban strategy maps	No, although DALES was successfully implemented, the progress in this direction was not sufficient. Instead, the case of using improved a-priori methane emissions for inversion of urban emissions was worked out further with a manuscript in preparation (planned to be submitted in January 2021).

Realized contribution to new knowledge and technology

The project has strengthened the knowledge and technology within TNO for high resolution air quality modelling through improvements in:

- General:
  - Increased understanding of the technologies used within TNO and the state-of-the-art outside TNO
- Spatially and temporally explicit emission modelling
  - Bottom-up traffic emission calculations
  - Update of Methane emission variability from agriculture
- High resolution dispersion modelling
  - Gaining experience with setting-up and using DALES
  - First insights in landscape scale dispersion characteristics

This research project has strengthened the technology position of TNO through starting the use of DALES in its atmospheric modelling portfolio. In addition, we have strengthened our position with respect to regional GHG inversions through the demonstrator application resulting in a scientific paper. Furthermore, the application of detailed traffic emissions is linked to a Brains4Nitrogen initiative, whereas the increase in resolution will be relevant for addressing nitrogen deposition policies in the future. Finally, the seed-ERP has given us the opportunity to design a roadmap aiming to fundamentally increase the resolution of the modelling systems at TNO, which will be pursued in the coming years.

Realized contribution to the market position

Dynamic anthropogenic emissions are key for assessing the importance of different sectors, identification of viable mitigation options and assessing the impact of transition scenarios or modal shifts. Modelling applications aimed at source apportionment, forecasting and emission monitoring, a core market of TNO CEE and T&T, rely critically on high quality emission data. In this starting phase we aim to cooperate with national (WUR, CBS, RWS) and international experts on activity and emissions modelling. By incorporating all sectors in a single system we aim to continue and expand our role as a key partner for emission provision in Europe and build the tooling required to do this at very high resolution for the Netherlands and any urbanized region in and outside Europe.

In 2020 we made the DALES system operational at the TNO HPC system and performed initial calculations for road and point source dispersion. Hyper local air quality modelling with Large Eddy Simulation (LES) models will be applied in the future to calculate high resolution air quality and urban climate studies, enabling to address

also spatial planning and biobased solutions. Outside the environmental realm, high resolution atmospheric turbulence and composition can be applied to optical signal propagation for detection and communication purposes. With the demonstrator and networking, we qualified ourselves for contributing to research programs in the abovementioned directions with this new functionality.

The literature reviews, strategy discussion and demonstrator activities have led to an improved insight in key development directions and improved awareness of expertise of the involved institutes, allowing a more targeted market approach in e.g. European project proposals on topics as novel methods to assess personal exposure, for studying the effect of mitigation options on hyperlocal air quality or for assessing the origin of nitrogen deposition. For the latter we also anticipate on a national knowledge program on monitoring nitrogen deposition with all relevant Dutch institutes to start in 2021.

Related projects in 2021:

Project / Activity	Type	kEUR	Project description
Knowledge programme on monitoring nitrogen deposition	B2B	200-400	Ensemble modelling for monitoring nitrogen deposition. We are currently involved in discussions related to the setup of this knowledge programme.
Postdoc Emission modelling methane	In-kind	-	Postdoc at the FUB (Freie Universität Berlin)

In this year a business plan has been developed for the ERP project. The first phase of activity on the market is to raise awareness by networking and knowledge sessions. In 2021 we will assemble a stakeholder group to take them along in the development of the model system and its applications. Envisioned stakeholders are (regional) governments, research institutes and NGOs. Where possible, additional funding (matching) will be attracted to strengthen the ERP. We aim to acquire related projects and cooperation's of the same size as the ERP project in 2021 (multiplier of 2). For example, we will tender for related Green Deal projects, or seek cooperation (e.g. post-doc positions), of which the results can be used in the new model system. We will formulate a dedicated action plan for attracting additional funding early 2021 together with Business Developers from the TNO units involved.

For the advancements made in modelling software and emission information we follow a strategy in which basic versions are open source and dedicated additions and base layers remain at TNO.

Publicity

Conference and workshop presentations

- Super, I., Dellaert, S., Visschedijk, A., Denier van der Gon, H., Schaap, M., Uncertainties in a high-resolution gridded emission map and the importance for urban scale emission verification, Presentation at the 2020 ICOS Science Conference, Online, 15-17 September, 2020.
- Schaap, M. Black Carbon (BC) in Germany: Improving spatial and temporal emission variability to improve source apportionment, Freiburger Workshop "Luftreinhaltung und Modelle", Online. 4 Nov. 2020.

Publications in preparation and submitted

- Super, I., Dellaert, S.N.C., Tokaya, J.P., Schaap, M., The impact of temporal variability in prior emissions on the optimization of urban anthropogenic emissions of CO2, CH4 and CO using in-situ observations, Manuscript in preparation for submission to Atmospheric Environment
- Ge, X, Schaap, M., Voogd, J-C,, de Vries, W., Detailing the Modeling of Atmospheric Ammonia for the Netherlands Using Sentinel-2 Derived Crop Map and Livestock Housing Information, Manuscript in preparation for submission to Atmospheric Environment
- Khan, B., Banzhaf, S., Chan, E. C., Forkel, R., Kanani-Sühring, F., Ketelsen, K., Kurppa, M., Maronga, B., Mauder, M., Raasch, S., Russo, E., Schaap, M., and Sühring, M.: Development of an atmospheric chemistry model coupled to the PALM model system 6.0: Implementation and first applications, Geosci. Model Dev. Discuss. [preprint], https://doi.org/10.5194/gmd-2020-286, in review, 2020

21 SEED ERP Circular Structures

ERP Contacts: Francesco Cinquini (Project Lead), Agnieszka Bigaj van Vliet (Lead Scientist), Arjen Adriaanse (Science Director)
ERP Duration: 2020 → Promoted to Full ERP

Progress 2020

Objectives

Climate change and the depletion of raw materials compel us to radically rethink our relation to the environment. On November 28, 2018, representatives of the EU presented their strategic long-term vision for a prosperous, modern, competitive and climate-neutral economy by 2050. To facilitate this strategy, in 2021-27 the EU will devote one-fourth of its budget to climate change policies (EU budget for the future : the new LIFE program - investing more in environment and climate action, 2018). By doing so, Europe will lead the way to climate neutrality by investing into realistic technological solutions, empowering citizens, and aligning action in key areas such as industrial policy, finance, or research. The construction sector is expected to deliver a substantial contribution to climate neutrality and sustainable development.

The current deadlock in enabling sustainable development of construction sector is largely caused by the major industrial challenge in the construction chain: the lack of integration of the CDW supply with the available design strategies for building structures. Considering that concrete structures are representing a vast majority of all structures being built, the solution to enabling sustainable development of building environment is to seek a paradigm shift in the design and production of concrete structures. In the life-cycle design of concrete structures, the requirements are imposed by the demands of safety, economy, and environmental performance. This leads to a multi-objective problem since these requirements are usually in conflict with each other. Development of trade-off solutions and selection of the optimum for implementation is very complex and efficient multi-objective design strategies are not yet available for concrete structures.

The breakthrough proposed in the project is to develop knowledge and technology that enables for concrete structures a shift from traditional design strategies to a new engineering design method driven by supply quality-demand integration. That goes beyond the current state-of-the-art performance-based life-cycle design (in which TNO holds a front-runner position). This breakthrough is achieved by setting short and long term objectives along three related research lines, each focusing on one aspect of the overall concept. The short term objectives described below are for the KIP of 2020; long-term objectives are included for giving an outlook to an overall 5-year ambition:

- *Research line 1* focuses on supply quality enhancement: the long term objective is to get the maximum value out of CDW for enabling low CO2 binders and reuse in concrete by developing activation & binder technology using the principles of molecular dynamics in both inorganic and organic chemistry. The short term objective for 2020 is development of a theoretical hypothesis on required molecular structures and organic-inorganic interactions as well as to obtain experimental evidence of these interactions in order to assess the feasibility and concept of using organic additives for enhancing the reactivity of inorganic CDW in binders.
- *Research line 2* focuses on supply quality-demand integration: the long-term objective is to develop a toolkit for CDW supply quality assessment by integrating both measurement and sensor techniques with performance models to enable a comprehensive quantification of quality parameters of CDW in relation to performance demands in life-cycle design. In the (multi-year) project this is done for all R-levels of circularity, from entire concrete structures over structural components to crushed rubble. The short term objective for 2020 is to assess the feasibility of developing and operationalizing a toolkit for quality assessment incl. integration of performance models & measurement tools.
- *Research line 3* with design driven by supply quality-demand integration, aims to develop a multi-objective multi-parametric design method for civil structural problems needed to enable optimal design based on integration of supply quality parameters (multi-parametric) and multi-objectives (criteria) of structural safety, sustainability, and costs. In 2020 the research aims to demonstrate the feasibility of multi-objective supply driven parametric design for sustainable concrete structures with output from the other two research lines, namely the envisioned quality requirements, tools and performance models.

During the (multi-year) project the total concept of the integrated approach shall be demonstrated for a number of relevant use cases showcasing how the proposed design method driven by supply quality-demand integration can be implemented in structural design to obtain optimum safety, sustainability and cost in life-cycle perspective.

Results realized

No.	Results planned	Realization
1	A list of requirements and candidates for bio-additives for activation in relation to CDW characteristics	*Yes (reported in TNO 2020 R 11891)*
2	Feasibility and concept for designing a durable and sustainable binder system based on CDW	*Yes (reported in TNO 2020 R 11891)*
3	Methodology for calibration of safety formats and modification of performance models for structural design with new solutions	*Yes (reported in TNO 2020 R 12291)*
4	Blueprint for integration of performance models & quality data based	*Yes (reported in TNO 2020 R 12291)*
5	Proof of Principle of sustainable design of concrete structures (aimed at minimising depletion of natural resources, CO2 emission and LCC) using optimisation algorithms in EVEReST	*Yes (reported in TNO 2020 R 12288, including demonstration of PoP in case study)*

Realized contribution to new knowledge and technology

Supply quality enhancement: In SEED ERP 2020, a molecular approach was formulated to design concrete binders based on CDW as such, instead of the trial-and-error approach used so far, which has led to firm conviction in the market that replacement cannot be done at high levels. The results of the SEEP ERP 2020 have proven otherwise. This approach enables faster steps in concrete binder development with larger replacement levels and enables to model and integrate quality parameters in sustainable design optimization. It was found that adding other inorganics (30%) combined with CDW is promising; but regulation of Ca-release is critical and requires organic additives. Thus, it was shown that the long term ambition of ERP (50% cement reduction) is feasible but methods are needed to quantify critical (in)organic additive dosages and parameter(s) for quality control and design optimization. Collaboration has been established with TU Wageningen, which provided organic additives for testing, and with TweeR Recycling, who tailored ultrafine CDW for quality enhancement.

New generation quality-based parametric performance modelling (structural, environmental, economic): In SEED ERP 2020, the safety framework currently used for modeling and design of new structures has been reviewed and adjusted for circular solutions to account for quality data and uncertainties of crushed CDW & components. The effect of the percentage of recycled CDW material in the concrete mix on the uncertainty of the concrete strength and structural performance has been described. With respect to the reuse of structural elements, the safety framework has been updated for uncertainties of properties and structural resistance based on the element material and structural testing. Methodology has been proposed for integration of quality data in resistance and durability evaluation of concrete structures with circular solutions. Next, an rout for improved approach to account for circularity and reuse in the environmental models has been set. Finally, an extension of the social impact model has been proposed by including newly formulated model for social satisfaction with regard to structural performance. This opens possibilities to achieve a major breakthrough by linking supply quality & uncertainties to parametric performance models used in structural design.

Multi-objective optimization of design of sustainable structures: In SEED ERP 2020, the technical, societal, environmental and economic performance aspects were evaluated simultaneously during a simulated design process using an adopted tooling for multi-objective optimization and decision support. Collaboration has been established with the University of Barcelona (Prof. A. de la Fuente) with regard to defining a sustainability framework for buildings and infrastructures. The suitability of state-of-the-art methods for multi-objective optimization under uncertainty for sustainable design of concrete structures was assessed. For demonstrating the feasibility of the multi-objective optimization, a case study was defined, performance models selected, and the optimization process was formulated with limited parametric variability. Implementation in multi-objective optimization tool showed convincing results in terms of an improvement of the (re-)design solution. For the multi-objective optimizations, TNO EVEREST and the open source jMetalP tools were used. Proof of principle demonstration in a case study (for crushed CDW and reclaimed elements in building floor structures) showed that the long term ambition of ERP (implementing parametric models in multi-objective optimization tooling) is feasible, while there is room for improvement with regard to dealing with increasing complexity of models and with regard to including risk-awareness in decision making.

This Knowledge Investment Project (KIP) significantly contributes to the improvement of the technology position of TNO by filling knowledge gaps in enabling sustainable development of built environment. The main objective of this project – providing innovative technology for creating a sustainable built environment - is the cornerstone of the Roadmap Construction and Infrastructure. The results contribute to achievement of the milestones of PMC cluster Infrastructure & PMC cluster Buildings, and in particular with the objectives of PMC Concrete Structures and PMC Building Materials. Research development and required expertise in this project are further aligned with that required for Roadmap Circular Economy (Circular Building: Next Generation Impact Assessment - development of learning curve methodology for innovations) and Roadmap CO2 neutral fuels & feedstock (development & adaptation of multi-objective multi-parametric design tools which incorporate any type of uncertainty prevalent in the system).

Being able to test and model performance of concrete structures with circular material solutions will speed up implementation of innovation in the field of material technology for concrete structures as it is prerequisite in advising both market parties developing new material solutions and owners allowing for application of innovative materials. New insights into use of multi-objective optimization in parametric design in combination with novel approaches to modelling performance of structures and its environmental and economic quality will make the TNO knowledge more relevant for dealing with the questions regarding design of circular structures. Knowledge development regarding effect of material quality on structural performance and on durability of concrete structures will allow for less conservative design and give basis for maximizing use of construction and demolition waste (CDW). Additionally, this knowledge is necessary in order to set standards for design of circular concrete structures and TNO has an ambition to play an important role in this process at that national and international level.

Last but not least, due to attention given to the use of material quality data, the project is complementary to other R&D of TNO and creates a broad basis for providing solutions aimed at enabling implementation of innovative digital solutions in built environment. Finally, with this future-oriented research focus the technology position of TNO is enhanced in such a way that we are becoming the most interesting knowledge partner for national and international (bilateral) collaboration and H2020 projects.

There is a rapidly increasing interest at Rijkswaterstaat and other public and private owners of buildings and infrastructure as well as market parties offering design and construction service to apply innovation in order to make a step change needed for reaching sustainability goals set in the Climate Accord. Climate change and the depletion of raw materials compel us to radically rethink our relation to the environment. On November 28, 2018, representatives of the EU presented their strategic long-term vision for a prosperous, modern, competitive and climate-neutral economy by 2050. To facilitate this strategy, in 2021-27 the EU will devote one-fourth of its budget to climate change policies (EU budget for the future : the new LIFE program - investing more in environment and climate action, 2018). By doing so, Europe will lead the way to climate neutrality by investing into realistic technological solutions, empowering citizens, and aligning action in key areas such as industrial policy, finance, or research. Following the Paris Agreement, in the Netherlands the government-wide Programme for a Circular Economy, entitled 'A Circular Economy in the Netherlands by 2050', was presented in 2016 and in 2018 the Dutch Transition Agenda for A Circular Economy has been set up.

The construction sector is one of the five key sectors which are being addressed and the challenges are huge: 50% reduction of primary resources and 50% CO2 reduction by 2030. Since 50% of the built environment consists of concrete structures, reducing the use of cement (responsible for app. 3% of the Dutch CO2 emissions) and other primary raw materials in concrete will have a massive contribution to solving these challenges. This is acknowledged by the construction sector and government who have launched the Concrete Agreement (Betonakkoord, 2018), additionally declaring that by 2030 all construction and demolition waste (CDW) from existing concrete structures must be used in new concrete. Yet, only 2% of the 22 Mton/year of CDW being released is reused in new concrete (the total Dutch concrete production amounts to 33 Mton/year).

The solutions develop in this project facilitate implementation of various circularity scenarios (including those related to recycle and reuse of concrete made from construction and demolition waste and reuse of reclaimed concrete elements) and are therefore straight forward relevant for reaching the aims of the Concrete Agreement (Betonakkoord, 2018). As the technology developed aimed at in this project is to large extend relevant for other types of materials and structures, the impact of this developments is potentially much larger. This aspect is being explored during the project activities with regard to recycling of demolition waste from wind turbine blades in concrete structures.

Realized contribution to the market position

The TNO portfolio will be significantly enlarged and increasingly attractive for stakeholders such as Rijkswaterstaat, Prorail and other public owners of buildings and infrastructure, who are governing large parts of the dedicated government funding for Transition Agenda (23 MEuro in 2020). Next, the TNO portfolio can be extended by attracting recycling companies, contractors, engineering companies and private owners of buildings, focusing on their circular transition. Importantly, the knowledge and tools developed for concrete structures, are a valuable basis for addressing circularity in other domains of construction industry.

Commercialization is at present considered for Rijkswaterstaat (with particular reference to the ongoing RWS SBIR call for Circular Viaduct https://www.tenderned.nl/tenderned-tap/aankondigingen/186605) which seeks to develop validated solutions for circular viaducts that can be repeatedly purchased and applied in (replacement and renovation) projects of Rijkswaterstaat, as well as in projects of other (semi-) public organizations and / or private parties in the Netherlands and abroad. Next, intensive contacts are ongoing and will be continued with the recycling companies and material producers (in 2020 with TweeR frontrunner in ultrafine CDW separation) and contractors (Lagemaat) aimed at attracting their attention to the technological development related to enabling use of CDW in new structures. Commercialization is also explored for the engineering companies with regard to design optimization solutions (in 2021 with Arup and RHDHV) and with providers of condition

assessment and material testing services with regard to design solutions enhanced with the quality measuring data (in 2021 with Nebest and SGS Intron). In mid-term perspective, results of the research will be implemented in guidelines and standards for design, assessment and monitoring of infrastructure, which include already initiated routes at fib, RILEM and CEN and expected shortly R&D under framework of BTIC and CROW/BTIC.

No specific actions on protection the results are being undertaken in 2020. In long-term perspective IP protection may apply to activation with bio(waste) additives, transferrable to other secondary resources.

Publicity

Publications

- Garzón Amórtegui, J.F., Batch dissolution test, paste test and mortar test for Construction and Demolition Waste (CDW) of concrete and brick, TNO-rapport TNO 2020 R 11869, 2020.
- Visser, J.H.M., Strategies to activate Concrete Construction and Demolition Waste (CDW) as binder in circular concrete, TNO-rapport TNO 2020 R 11891, 2020.
- Allaix, D.L., Bigaj-van Vliet, A.J., Heinemann, H.; Valcke, S., Methodology for adjustment of safety formats and performance models and use of quality data in design, TNO-rapport TNO 2020 R 12291, 2020.
- Valcke, S., Bigaj-van Vliet; A.J., Allaix, D., S., Rozsas, G. Martini, A., Fonseca, R., Godoi-Bizarro, D., Hauck, M., Visser, J.H.M., PoP Sustainable Design of Circular Concrete Structures, TNO-rapport TNO 2020 R 12288 2020.
- Valcke, S., Kruithof, J., Route naar circulair beton, presentation in IQ-stuurgroep meeting, 11 September 2020.
- Valcke, S., Circulair beton & betonconstructies - actueel & toekomstbeeld, RWS Kennislezingen, 29 October 2020.
- Bigaj-van Vliet, A.J., Structural safety of concrete structures in changing construction world, presentation in fib Webinar Latest Developments, https://www.youtube.com/watch?v=PJs2vXJ5tFg, 25 November 2020.
- Valcke, S., Circulariteit in beton & betonconstructies - actueel & toekomstbeeld, Lagemaat stakeholder gesprek, 11 December 2020.

22 SEED ERP Solar2Hydrogen

ERP Contacts: Nicole Meulendijks (Project Lead), Pascal Buskens (Lead Scientist), Christa Hooijer (Science Director)
ERP Duration: 2020

Progress 2020

Objectives

Hydrogen (H_2) is currently used at a scale of ca. 70 Mt/yr, predominantly in chemicals production and refining. The majority of H_2 produced today is from fossil fuels and causing around 830 Mt/yr of CO_2 emissions. (Inter-) national targets regarding CO_2 emission reductions alongside increasing renewable energy (RE) supply, require innovation in terms of RE storage and conversion. RE-driven electrocatalytic water (H_2O) splitting to produce H_2 may become attractive as low emission fuel for mobility and heat supply, as energy storage vector, and as industrial feedstock (e.g., sustainable ammonia production, CO_2 conversion to platform molecules) (see *Figure 19*). The role that H_2 can play in a sustainable energy system and its supply chain versatility has attracted stakeholders from different sectors to explore the possibilities.

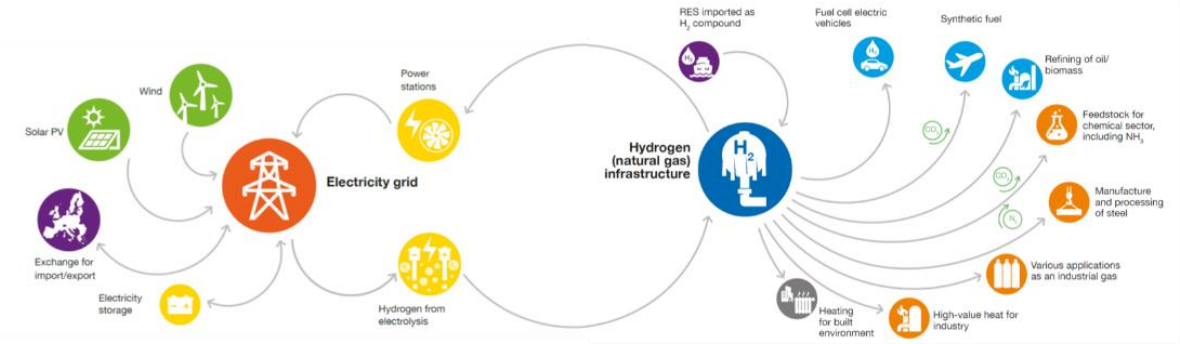


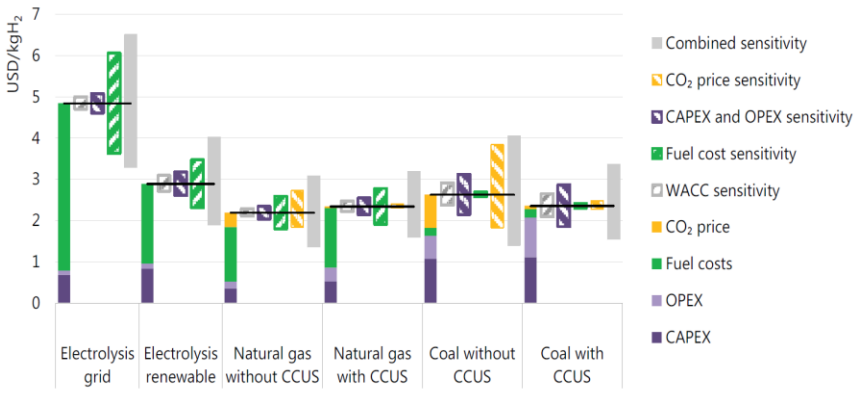
Figure 19: System function of H_2 in a sustainable energy and raw materials landscape[10].

Current H_2 production costs range from 1-2 €/kg from natural gas to 4-5 €/kg from grid electricity. To reduce CO_2 emissions, H_2 produced with electrolysers is ideally powered by RE for instance by photovoltaics (PV). Although substantial cost reductions for both PV and electrolysers are expected, production costs of around 3 €/kg(H_2) are projected for 2030 (depending on the scenario).[11][12] Technologies that enable to produce renewable H_2 at even lower costs would be highly interesting.

Significant improvements are still required if the cost of H_2 production from these technologies is to be competitive with H_2 produced by conventional (fossil fuel-driven) technology. In this regard the prognosis as highlighted by Detz *et al*., shows that the most novel technologies (e.g. of the cell type proposed herein), if optimistic assumptions are taken, may become competitive in a relatively short time frame. PEC cells with their expected high Learning Rates (LR) (e.g. as observed from conventional PV technologies) and Compound Annual Growth Rates render these tech options particularly susceptible to rapid cost reductions. A disadvantage of these routes is the relatively low Capacity Factors of only *ca*. 20%, as well as the high initial investment costs – therefore production methodologies that help to address this point are needed. Going forward, provided investment costs become low enough, PEC devices will become increasing interesting – they must therefore be rapidly accelerated in terms of TRL and raise them quickly to production (e.g. beyond the existing demonstrators).

[10] J. Ikaeheimo J.Kiviluoma R.Weiss, H. Holttinen, Int.J.Hydrogen Energy, 2018, 43, 36, 17295
[11] https://webstore.iea.org/the-future-of-hydrogen International Energy Agency Report, 2019, "The future of hydrogen – seizing today's opportunities"
[12] G. Glenk, S. Reichelstein, Nature Energy, 2019, 4, 216

One technology concept which has the potential to produce renewable H_2 at a lower cost price than electrolysis is the so-called 'Solar2Hydrogen' concept. This field of research is still in an early phase and "lab-scale devices" have been demonstrated, mostly by academic research groups, at TRL < 5. The most developed setup consists of a PV cell, directly wired to two electrodes that should split the H_2O, leading to high Solar-to-H_2 (STH) efficiencies (> 15%). Different levels of PV and electrolysis technology and material integration have been discussed in the literature (e.g. via solar concentrators; (see Key Literature sources for reference information).



Notes: WACC = weighted average cost of capital. Assumptions refer to Europe in 2030. Renewable electricity price = USD 40/MWh at 4 000 full load hours at best locations; sensitivity analysis based on +/-30% variation in CAPEX, OPEX and fuel costs; +/-3% change in default WACC of 8% and a variation in default CO_2 price of USD 40/tCO_2 to USD 0/tCO_2 and USD 100/tCO_2. More information on the underlying assumptions is available at www.iea.org/hydrogen2019.

Projected costs of H_2 production in 2030 from the IEA.

Perhaps the most prominent example has been reported very recently by KU Leuven, who reported on a solar device that converts H_2O vapour into H_2 and O_2 (250 L/day) at a STH efficiency of 15%. Challenges regard longer term device use due to electrocatalyst degradation under dynamic RE loads. A potentially more elegant approach to PV+EC, involves the design, integration and operation of device composed of a PV unit interfaced directly within one cell module to an electrolysis stack (denoted hereon as integrated PVE for integrated photovoltaic electrolysis). This integrated PVE approach, although currently less developed with regard to TRL (e.g. in comparison to PV+EC), has a number of potential advantages. Delivery of H_2 off-site (e.g. via gas pipelines) is potentially less expensive than the transportation of electrons via conventional electrical grid cabling. Furthermore, the integration of PV and electrolyser units in one PVE device has the potential to improve overall H_2 production efficiency (and in turn reduce H_2 production costs). This integration is also potentially beneficial with regard to land area use and reduced system footprint. An example of a proposed integrated PVE device would consist of layers commonly observed in the architecture of a 2T tandem PV cell (e.g. a Silicon HeteroJunction (SHJ) cell combined with a perovskite-based top-cell – theoretical electric efficiency of *ca*. 24%). In this respect, combinations of photoactive materials can be employed to achieve an operating voltage of *ca*. 1.6 - 1.7 V. This 2T cell configuration can then be coupled to the electrolysis unit, which can achieve a solar-to-H_2 (STH) efficiency of approximately 17% if H_2O splitting is matched to the current of the PV cell at a voltage of 1.7 V.

Regarding the electrolysis component, H_2O splitting can be performed under either acidic or alkaline conditions (each bringing their associated benefits and challenges). Under acidic conditions, the cathode (where the Hydrogen Evolution Reaction proceeds) is interfaced at SHJ bottom of the PV cell via a conductive and porous transport layer, which conducts electrons from the solar cell to the cathode/electrocatalysts, transporting the evolved hydrogen away from the cathode (e.g. via an appropriate porous material). The cathode is connected via a proton exchange membrane (PEM; typically polymeric) to the anode. At the anode, water oxidation occurs as electrically connected to the top-cell (closing the electrical circuit). H_2O is supplied to the anode via a porous transport layer, which facilitates the evolving O_2 to escape the system. Operation under alkaline conditions is attractive as it allows less expensive electrocatalysts to be used (e.g. Fe/Ni vs Ir/Pt). This is an important consideration with regard to commercial deployment. Likewise in both setups, water management and by implication the function/efficacy of the thin transport layers becomes of critical importance and a key area of investigation. Regarding overall PVE unit integration, connections and sealings are important components in the assembly. Therefore, the successful establishment of a Technology Roadmap for the production of the proposed integrated PVE devices initially aiming at TRL4-5, as supported by techno-economic validation, will support the delivery of scalable integrated PVE devices in the longer term. The roadmap includes a number of challenges concerning module operation, design, and fabrication, which must be overcome if economically viable H_2 production is to be achieved. Suitable materials are needed for the capture and conversion of the

incident photons. In PV, current can be exchanged for voltage, so materials with a relatively wide range of band gaps can be used to produce mutually similar net electrical power as the system output. With respect to the 2T cell type described briefly above (and perovskite-based cells in general), it is important to consider cost, sustainability, and stability of the solar cells.

Regarding electrocatalysts, these must be highly active, stable, and, for global scalability, must be either comprised of earth-abundant elements or must minimally utilise scarce metals (e.g. Ru or Ir). Currently, the most active catalysts for water splitting (under acidic conditions and high TRL) are Pt and IrO_2. Therefore, there is a need to develop alternative electrocatalysts ideally based on more common, less expensive transition metals, alloys thereof or oxides (e.g. Mo, W, Co, Ni, Fe, or Mn; as nanoparticles or molecular species). This challenge is further complicated by the need to operate both the oxidative and reductive electrocatalysts under mutually compatible conditions of pH, temperature, *etc*.. Then the electrolyser unit also needs to be interfaced with the PV unit, while retaining as an assembly the function of all of the individual pieces. In this regard design and selection of membranes and porous transport layers are critical to provide efficient operation (e.g. inhibiting back diffusion). The system must allow a facile, low-resistance path for ion (generally H^+ or HO^-) conduction to neutralise the pH gradient, else the net reaction to form products will cease to occur. For this reason, suitable membranes or alternative physical/chemical/mechanical product separation schemes a critical to achieve a scalable integrated PVE device.

Large scale production of the proposed integrated PVE devices should draw on the experiences of mass fabrication technologies (e.g. roll-to-roll manufacturing) and that of large scale manufacturing of PV technologies. Given the initial design proposition of the integrated PVE device above, synthetic techniques such as Atomic Layer Deposition or Layer-by-Layer (LbL) assembly as scaled-up to roll-to-roll processing are already used in industrial production of millions of m^2 per year. Experience from the use of these approaches in a range of applications (e.g. PV, optoelectronic devices, energy storage, coatings, microreactors, flexible electronics) can be co-opted to assist to enable production of PVE devices.

The aim of the Seed-ERP project is to consider the manufacture of a fully integrated H_2O conversion device in which light harvesting, charge separation, and catalysis can be unified to produce H_2 in a single step, thus leading in turn to low(er) investment costs. Regarding LR, know-how and indeed experience can be gleaned from the production of analogous integrated systems, such as PV cells for the production of electricity, which have rapidly reduced in cost over the last 20 years. Therefore to further facilitate progress in this field, lab-scale devices have to be scaled-up to cell and module size, whilst being preferably constructed with inexpensive and abundant materials. To do this in an efficient manner, a substantive Technology Roadmap is required.

As highlighted the design of a potential integrated device within the scope of this KIP will require know-how from various fields of expertise from within TNO. In this regard competences relating to material chemistry (e.g. light absorbers, catalysts, electrolytes, membranes etc.) will be strongly required as will be competences relating to the processing and assembly of the material components necessary to complete and operate the cell. In this context expert colleagues from Solliance have a strong track record regarding the technological challenges of synthesising and processing of materials for PV technology, from the fundamental aspects to the analysis and scale-up phase.

Concerning the unit Industry, research is strongly focusing on the development of catalytic technology suitable to facilitate the conversion of electrical and photonic energy into chemistry and fuels (e.g. *Electrons-to-Fuels, Photons-to-Chemicals lines of the ERP-ESC*). Here existing competences are to hand regarding catalyst selection, synthesis and design. Contributions in this regard are already being made within the VoltaChem program (e.g. *Electrocatalytic conversions; Power-to-Hydrogen; Power-to-Specialities etc*.). From the ETS group, extensive knowledge and background exists with regard to the techno-economic and environmental assessment of renewable energy technology, materials and chemistry.

Deliverables 2020

1. Development of a lab-scale prototype for ‘solar-2-hydrogen’, which demonstrates that TNO houses the competences and infrastructure to develop and study materials and devices for ‘solar-2-hydrogen’.
2. An economic analysis of a range of ‘solar-2-hydrogen’ concepts, to demonstrate the future potential of producing renewable H_2 at a cost price below 2 €/kg.

3. Development of a technology roadmap for the development of technically and commercially attractive PVE devices up to TRL 4-5, as basis for a full scale ERP program.
4. Mapping of academic research groups active in 'solar-2-hydrogen', focussing primarily on The Netherlands and Flanders.

Key Background Literature

1. "Towards Practical Solar Hydrogen Production – An Artificial Photosynthetic Leaf-to-Farm Challenge", Jang, Lee, et al., Chem. Soc. Rev., **2019**, 48, 1908
2. "Concepts of Photoelectrochemical Energy Conversion and Fuel Generation", Lewerenz, Sharp, Ch. 1, p. 1-42 in "Integrated Solar Fuel Generators"; Editors: Sharp, Atwater, Lewerenz, Royal Society of Chemistry (UK), Cambridge, UK, **2019**.
3. "The future of solar fuels: when could they become competitive?", Detz et al., Energy Environ. Sci., **2018**, 11, 1653.
4. "The Artificial Leaf" Nocera, Acc. Chem. Res., **2012**, 45, 767.
5. "Opportunities to Improve the Net Energy Performance of Photoelectrochemical Water-splitting Technology", Sathre, Greenblatt, et al., Energy Environ. Sci., **2016**, 9, 803.

Key Literature regarding PV and Electrolyser Integration

1. "*Solar water splitting by photovoltaic-electrolysis with a solar-to-hydrogen efficiency over 30%*", Jaramillo *et al*., *Nat. Commun.,* **2016**, 7, 13237 – STH% = 30.0 (notably low level of PV and PEM electrolysis cell integration; tested only over a 48 h operation window)
2. "*Water photolysis at 12.3% efficiency via perovskite photovoltaics and Earth-abundant catalysts*", Grätzel *et al*., *Science*, **2014**, 345, 1593 – STH% = 12.3 (perovskite PV interfaced with AEL electrolysis; PV materials limit cell lifetime whilst AEL use under dynamic loads (i.e. degradation rates) not addressed).
3. "*Recent development in direct generation of hydrogen using multi-junction solar cells*", Ohlmann *et al*., *AIP Conference Proceedings*, **2016**, 1766, 080004 - STH% = 34.2 (Complex GaInP/GaInAs dual-junction PV interfaced with PEM cell; solar light concentrated using Fresnel lenses) – further elaboration of a previous report "*Solar hydrogen production by water splitting with a conversion efficiency of 18%*", Dimroth *et al*., Int. J. Hydrogen Energy, 2007, 32, 3248 (STH% = 18).
4. "*Renewable fuels from concentrated solar power: towards practical artificial photosynthesis*", Wiechen, Spiccia *et al., Energy Environ. Sci*., **2015**, 8, 2791 – STH% = 22.4 (Modular approach based on commercially available GaInP/GaAs/Ge multijunction PV and AEL; query regarding long term operation under dynamic solar loads).

   "*Designing a hybrid thin-film/wafer silicon triple photovoltaic junction for solar water splitting*", Perez-Rodriguez *et al., Prog. Photovolt. Res. Appl*., **2019**, 27, 245 – STH% = 8.3 (stable over 10 h; integrated device featuring hybrid thin-film/wafer silicon triple PV junction coupled electrically with a IrOx/Pt based PEM electrolyser).

Results realized

No.	Results planned	Realization
2	Economic analysis of a range of Solar2Hydrogen concepts in comparison with electrolysis	yes
3	Inventory of academic stakeholders involved in Solar2Hydrogen in Flanders and Netherlands	yes
	Reports, papers, presentations planned	
1	Report/paper concerning Solar2Hydrogen techno-economic analysis	In progress, expected Q1/2 2021
2	PowerPoint slide deck presenting the project results	Yes
3	Workshop/discussion session with internal/external experts	Yes

Realized contribution to new knowledge and technology

Within the project H2 producing cell concepts that feature increasing degrees of light harvesting and water splitting technology integration in tandem with cost effective, scalable fabrication techniques, with the aim to deliver low cost, green H2 (vs. classical PV plus electrolysis) were explored.

Solar water splitting to produce H2 (and O2 as by-product) has been investigated for over 50 years but has received more extensive interest in recent years. Globally, there are several players are active in this field, mostly at the academic level. These combined efforts have led to conversion lab-demonstrators with efficiencies of 2% (for photocatalytic), 8% (for hybrid PV-photoelectrochemical cells (PEC)), 19% (for buried junction PV) and even 30% (for PV coupled to electrolysers). Despite this work and prior art, significant improvements are still required if the cost of H2 production is to be competitive with fossil-based H2 production. In this context, the fabrication and demonstration of fully integrated, modular solar water splitting devices would represent an increase in Technology Readiness Level (TRL), adding value to the market and related TNO activities.

In the SEED-ERP a lab scale S2H demonstrator was fabricated, producing H2 based on an integrated hybrid PV-PEC concept. This and two other S2H concepts were techno-economically assessed to demonstrate the future (low) cost prognosis of producing H2 based on this technology. Top-down analysis reveals that devices could cost between 120 - 600 €/m2(device) enabling green H2 production at 2 €/kg. Based on a bottom-up system cost estimate, as complimented by existing literature, capital expenditures (CAPEX) was calculated as ca. 150 – 330/m2 (depending on exact device concept). The overlap between these projections reveals that low cost, green H2 production should be economically feasible and market competitive.

Realized contribution to the market position

Improvement of the market position of TNO (turnover, customers) by providing:

- Unique concept for photoelectrochemical water splitting.
- Economic analysis of a range of ‘Solar2Hydrogen concepts resulting in a technology roadmap for the development of technically and commercially attractive Solar2Hydrogen (and related PEC) devices up to TRL 4-5

The SUN-ERGY initiative was joined. At the moment the consortium is mainly in a lobby phase and they are trying to strengthen the consortium towards Horizon Europe. Partnership with the current affiliated parties is considered.

After analyzing the results, publishing in scientific journals have found more interesting and useful at this stage. In the coming year the patent strategy will be further defined.

Publicity

- A report/paper concerning the Solar2Hydrogen techno-economic analysis is currently being drafted, publication is expected Q1/2 2021
- Due to COVID not conference presentations could be held. The ongoing activities have been presented to a small group of researchers at Hasselt University and the University of Amsterdam to explore whether collaboration could be possible. This will be followed up in 2021.

23 SEED ERP Business Models for Transition

ERP Contacts: Hugo Gelevert (Project Lead), Frank Berkers (Lead Scientist), Anne-Fleur van Veenstra (Science Director)
ERP Duration: 2020

Progress 2020

Objectives

The central research question of this this SEED ERP was '*How can collaborative business models be used to shape and guide transition towards sustainability?*'. This leads to the following sub-questions:

1. **Design**. What are possible design parameters for collaborative business models and how to best typify these BMs and their interrelations with the different actors in the ecosystem (firm, government, non-government)?
2. **Transition routes**. What are possible transition routes, and which collaborative business models fit best with which routes?
3. **Scaling**. What are factors (institutional, economic, commercial, policy, etc.) enabling or hindering up-scaling, and which collaborative business models and transition routes can address these best?

Co-creation. How to shape co-creation of the design and development of collaborative business models with various actors? Including whom to engage, incorporating transition objectives, shaping individual and collective mindset-shifts and forthcoming organizational changes.

Results realized

The project was executed according to plan. There was one deviation: 1 single complete case study was not feasible as none of the identified cases was able to illustrate all desired aspects. The findings / results are described below:

Literature: scientifically new field

- Three academic papers in the making:
  - Scientific Paper CBM for inclusive innovation in collaboration with TU Twente en Nyenrode, een structured literature review, submitted bij IJManagement Review
  - Transition Pathways paper: Scientific paper reporting the overview and synthesis of transition concepts* drafted
  - CBM4T Paper*: Scientific paper reporting cross-case analysis, drafted (target Journal of Cleaner Production)
- MSc Thesis: T-pathways (RU)
- Working paper CBM4T: TNO report based on scientific literature on transition studies and business modelling and cases. Presented at the NBM conference
- Research agenda CBM4T: Identification of relevant fundamental and applied research topics for CBM4T in- and external consultation. Comprised in Working paper and full ERP proposal

Practice: unique TNO contribution

- CBM4T-program-quickscan was developed: Literature based aspects that an effective CBM4T approach should fulfil. Used to analyze cases. Also successfully applied in EN-ZUID
- +MSc Thesis: Analysis from CBM4T perspective of CiloLab case* (TU/e)
- Assessment of 41 transition cases: External and internal 'transition cases' meeting pre-set criteria
- Cross case-analysis for 3 cases: Description and analysis of cases: Samso, RESCO and CiloLab. Leading to identification of 5 Spearheads for CBM4T-methodology

Network: positioning TNO and CBM4T

- New Business Models international conference
  - NBM keynote: Director CEE (Marinke Wijngaard) explaining the CBM4T concept at NBM conference. Also, in LinkedIn post.
  - NBM session: Dedicated scientific session (and contribution) on business models for transition at NBM conference

    - NBM Track: 6 sessions devoted to tools in the TNO Sustainable Business Model Innovation framework, in collaboration with PACE and VITO
- Academic network established
    - Academic Network and conference: Selection of PhD candidates, researchers, professors on the intersection of TS and BM
    - Contact with 'Transition group' of Groene Brein (André Nijhof)
- YouTube movie, TNO position paper
    - YouTube movie: animation and explanation of the CBM4T concept (NL+EN). Included in CBM4T media campaign
    - TNO Position Paper*: Introduction and call to action for CBM4T (in Dutch)
    - External Collaboration: Academic Network (7), NBM Conference, PACE, VITO, Radboud, TU/e, CiloLAB, Resco, 5 municipalities

Realized contribution to new knowledge and technology

Transitions require participation and substantial change by businesses, yet the link between business modelling and transition studies is a clear scientific gap. Also, in practice there is little guidance for the development of business models that help organizations to make the shift from niche to regime at scale.

CBM4T has identified a full framework applicable to programs (aimed at innovation in sustainable transition) and pilots. This framework identifies key aspects that need be addressed on these levels. This work has shown 5 key principles that are currently weakly addressed in available approaches. These are: Scale and multi-value in focus from the on-set; 2. Creates 'window of opportunity' for niche innovations; 3. Destruction of existing regime to make room for niche innovations; 4. Clarity on system change required; 5. Need for a participative CBM-development methodology.

With its position in Sustainable Business Model Innovation, Transition Management and a strong foothold in many industries, TNO is in a unique position to organize and integrate these knowledge fields and make these applicable to the transition practice. In the Netherlands and beyond TNO has good relationships with regional and national governments that aim for transitions, and TNO also has good relationships with the universities and institutes that develop relevant knowledge. The CBM4T is a unique contribution to the Netherlands agenda on Key Enabling Methodologies.

The capability to involve businesses in transitions on a structural level is desperately needed and acknowledged from several ministries and regional development agencies, e.g. infrastructure, economic affairs, internal affairs.

Realized contribution to the market position

The proposition benefits the position of CEE, ET and SA&P to a large extent as regional clusters (HBR, BrightSite, etc.), regional development agencies and ministries are actively requesting this type of knowledge in programs and the Key Enabling Methodologies agenda.

Through Orchestrating Innovation, CEE and ET the team has access to large scale sustainability-oriented innovation programs, like EN-ZUID, BrightSite, CESI, and will introduce the program leaders into this proposition.

Publicity

Publications

- TNO 2020 R11009 Collaborative Business Models for Transition: http://publications.tno.nl/publication/34636797/vmt66M/TNO-2020-R11009.pdf
- YouTube, Collaboratieve Business Modellen: https://youtu.be/lt4tHhgRrho
- TNO 2020 R11638 Sustainable Business Model Innovation: https://bit.ly/TNOSBMI
- The contribution of Collective Business Models in enabling a Transition towards Sustainability – Gijs Kaal (Master's thesis)
- Transitioning towards Sustainable City Logistics through Multi-Stakeholder Interactions – Zebaish Masood (Master's thesis)
- TNO.nl: https://www.tno.nl/nl/aandachtsgebieden/strategische-analyses-beleid/expertisegroepen/strategic-business-analysis/collaboratieve-business-modellen/
- Elevator pitch: https://www.youtube.com/watch?v=lt4tHhgRrho&t=5s
- New Business Models Conference: https://www.nbmconference.eu/
- New Business Models Conference, keynote Marinke Wijngaard

24 SEED ERP Human Capital

ERP Contacts: Goedele Geuskens (Project Lead), Joost Van Genabeek (Lead Scientist), Paulien Bongers (Science Director)
ERP Duration: 2020

Progress 2020

Objectives

Our society faces grand societal transitions, such as the energy transition and digitalization & robotization. The major bottleneck in successfully realizing these transitions is no longer of technological nature, but concerns social innovation and behavioral change. To enable grand societal transitions, this SEED ERP focused on the necessary conditions for a dynamic skills-based labour market, a major transition and system change in itself. The reason is that our labour market is struggling with friction in demand and supply of work. This mismatch will increase due to transitions such as the energy transition and digitalization, as they will further change working tasks and create and destroy professions. The currently growing mismatch hampers the productivity and competitiveness of companies, and puts the realization of for instance climate goals at risk. In this fast changing world of work, it is crucial that workers continuously learn new skills to do their job (upskilling) or learn different skills to switch to another profession and sector (reskilling). The COVID-19 pandemic underlines this necessity of mobility. However, an effective system for up- and reskilling and intersectoral mobility is still lacking.

The fundamental transition to a **skills-based work-learn environment** requires extensive knowledge development in 3 domains. First, a common dynamic skills language, specific for the Dutch labour market, is needed as the fundament of the skills approach. It should be responsible, e.g. preventing discrimination. Second, skills-based instruments (e.g. assessment, matching, prediction, etc.) and interventions (in which the skills-based instruments are one of the elements) tailored to individual persons, organizations and contexts are needed. Third, to scale up effective skills strategies, empirically validated insight is required in how the skills approach fits into the system level (e.g. design current work-learn system, culture, funding, regulations and legislation).

This SEEDS ERP was our first step towards the development of skills based human capital strategies that enable grand societal transitions. More specifically, the objectives of this SEEDS ERP were:

- To study the (potential) value of a skills based labour market to enable grand societal transitions
- To contribute to the development of a dynamic skills ontology as the basis of innovative human capital strategies, in close collaboration with partners
- To (further) develop 1 or 2 use cases for grand societal transitions in which inclusive human capital strategies are created in close collaboration with private and public partners.

Results realized

No.	Results planned	Realization
1	Semi-static explainable responsible skills ontology based on data of existing expert systems	**Partly**. TNO performed the work on linking O*NET to ESCO/ISCO as planned, but manual checks on the crosswalk with O*NET still need to be carried out by UWV professionals. TNO is investigating whether a more precise crosswalk is possible with the help of NLP, which would reduce manual checks.
2	Approach to make semi-static skills ontology dynamic to changes in skills needs on our labour market	**Yes.**
3	Dynamic explainable responsible AI skills ontology that automatically adjusts to changes in skills needs on our labour market	**No**. The realization of this result was too ambitious. However, in addition to the development of the approach to make the skills ontology dynamic, a prototype was developed for automatic extraction of skills from vacancies. This methodology can be used to detect changes in skills demand on our labour market in future.
4	At least 1 use case: Agreement on needs, goals and conditions among stakeholders	**Yes**. In 2 use cases a skills based instrument was developed or studied, and in 3 additional use cases a broader skills based intervention was developed (design of concept, n=2) or studied.
5	At least 1 use case: Design of concept developed by stakeholders	

	Reports, papers, presentations planned	
1	Research report about the design, working and functionalities of the AI Skills ontology	**Yes**. A scientific paper on the development of the skills ontology based on existing classifications and a report on the architecture of a dynamic future proof skills ontology were written.
2	1 presentation on (international) conference	**Yes**. Presentation February 10th 2020 at ESCO-conference Brussels on skills-matching tooling using skills-taxonomies.
3	2 landmark publication on skills based approach/skills ontology, ready to submit Publication 1 ready to submit	**Yes**. One paper was submitted and accepted, the second paper (draft) will be submitted in the beginning of 2021.
4	Short report on use cases, describing needs, goals, conditions, design of concept, first indications of impact, and lessons learned	**Yes**. Instead of one short report, separate deliverables for all use cases were made (scientific article, report, PowerPoint presentation).
5	Roadmap and work plan of full ERP (2021-2023)	**Yes**. ERP proposal

Realized contribution to new knowledge and technology

New knowledge and technology acquainted includes:

- Improved knowledge on hybrid AI applied to skills ontologies and changes on the labour market.
- AI methodology to extract skills from vacancy texts.
- Improved knowledge on using a skills ontology as the fundament for skills based instruments applied in practise.
- Improved knowledge on how skills based human capital strategies can be developed in co-creation with partners in different sectors.

This contributes to the improvement of the technology position of TNO as follows:

- Understanding of ways for adapting knowledge models (such as existing skills ontologies) to a changing world (such as changes on the labour market).
- Basic skills languages have been developed, i.e. in the USA, at EU level, and in some European countries. However, no country has been able to bring these languages into life and establish a skills-based work-learn environment. The SEED improved our knowledge position on ***how*** a skills ontology can effectively be applied in practice and how skills based human capital strategies can be designed.

Realized contribution to the market position

Improvement of the market position of TNO

- UWV and CBS have a better view of how TNO can contribute to AI, which can be applied to UWV's application of CompetentNL. TNO and UWV (and CBS) discuss a long-term collaboration.
- Integrating AI, skills based instruments and interventions, and skills ecosystems in different sectors/contexts improved our position as a key player in studying and establishing a skills based labour market and enabling grand societal transitions. Both with respect to national (Bouwend Nederland, SBB, MBO raad, etc.) and regional stakeholders (e.g. industry, municipalities, education).

No efforts have been taken for commercialization of the results of this project.

Publicity

Publications

- Paper: J van Genabeek, S van den Heuvel, R van den Bergh, H Verhoef, K Kranenborg, G Geuskens. Een hulpmiddel voor het verkrijgen van inzicht in skills en bijpassende banen: Ontwerp, werking en gebruikersgemak van De Paskamer tool van House of Skills. *Accepted for publication*
- Paper: L Oosterheert, G Geuskens, J van Genabeek, J Tang, Developing dynamic skills classifications, using expert-based and data-driven approaches, *draft*
- Paper: S Vethman, A van Luenen, C Veenman, Skills-based job matching vulnerable to discriminatory practices, *draft*.
- Report: R van den Bergh, H Verhoef, E van Kempen, G Geuskens. Van Technologie naar skills en verwantschapsbanen: TOP aanpak. TNO, 2020.
- Report: E van Kempen, R van den Bergh, H Verhoef, G Geuskens. Impact van Connected Automated Transport op skills van vrachtwagenchauffeurs. TNO, 2020
- Presentation: J van Genabeek. Skills matching tooling using skills taxonomies. ESCO conference, 2020, Brussels.

25 SEED ERP Energy Modelling

ERP Contacts: Peter Mulder (Project Lead), Martin Scheepers (Lead Scientist), Andre Faaij (Science Director)
ERP Duration: 2020

Progress 2020

Objectives

After decades of relatively little change, the energy system is currently in a rapid transition that is not about to end soon. This is leading to profound and sometimes fundamental changes in energy infrastructure, generation and primary energy mix. Also the use of energy carriers in industrial production capacity, transport sector and built environment will change. With the energy transition progressing, impacts on the economy, society (e.g. jobs, income effects) on space, the use of (natural) resources and the environment increase, both in a positive (synergies) and negative (conflicts and constraints) way.

Decision makers in the energy system – ranging from (inter)national policy makers, via businesses to individual citizens – need reliable and up-to-date insights to base their policy and investment decisions upon. TNO already is an important party in providing these stakeholders with insightful analyses of possible energy futures. To generate these insights, we use a suite of energy models and methods on different geographical levels. Our stronghold is that we are able to study the dependencies in the energy system and to analyses the impact of decisions on the entire energy system, combined with profound technological know-how and interdisciplinary analytical capabilities.

The current suite of TNO energy models may benefit from much improved modelling capabilities and new insights on the following fields:

- Encompass geographical information on different scales (international – local), to be able to understand and analyze both spatial restrictions and spatial consequences and impacts of the energy transition and required energy generation capacity and infrastructures.
- Incorporate agent behavior (households, car owners , industries, investors, etc.) in energy models, covering different relevant dimensions (investment decisions, consumer preferences, risk perception and heterogeneity in stakeholder groups to name some important aspects).
- Technological progress and (rapid) learning of a large number of energy technologies that strongly affect business decisions and choices for infrastructures.
- Increased complexity in the energy system due to strongly increasing number of generators, energy system and sector integration with power to heat and PtoX options as well as flexibility and storage possibilities.
- Deep decarbonization of industry impacting value chains (i.e more circular) and industrial energy demand with combined with potential major effects on (macro-) economic structure.

SEED-ERP 2020 objectives: overview of modelling suite, development needs, state-of-the-art and run a case study on new tooling

The goals for 2020 are:

- A comprehensive overview of models relevant for the energy transition available at TNO, including their possibilities and limitations in relation to support decision making in the energy transition;
- An overview of the main new modelling capabilities and new insights, including perspectives to improve or supplement our modelling suite;
- Perform a case study in which we apply one or two new modelling principles in the field of heat supply.

Results realized

No.	Results planned	Realization
1	Internal report describing needs, current modelling base at TNO and the most important new modelling principles.	Yes
2	Draft publication on the heat supply case study	Yes
3	Plan for full ERP, including external funding opportunities.	Yes

Realized contribution to new knowledge and technology

In short, we concluded that the most important questions that TNO must be able to answer in the context of the energy transition over the next 5-10 years are these:

1. *Energy systems in the future:* What are the possible transition paths to a sustainable energy system for the Netherlands in 2050? How do you determine a no-regret strategy to realize the energy transition across the entire chain (generation, storage, conversion, transport, use? How do decentralized energy system choices and decisions impact the overall energy system as well as other domains, such as mobility, industrial transformation or the circular economy?
2. *The spatial dimension of the energy transition:* What are the spatial impacts of the energy transition for the way in which we organize the spatial domain? What conflicts does this cause? What restrictions and options for policy are there?
3. *Behavior and policy:* How can you use policy to speed up the implementation of the energy transition? How do you influence the behavior of companies and citizens in the desired direction with policy?
4. *The economic and social context of the energy transition*: What is the impact of the energy transition on housing, mobility and logistics, work, economic structure / production / employment, international trade / competitive position? Which economic and social developments (e.g. digital development, circular economy) should you take into account in the energy transition?

These questions relate to 4 areas for which TNO currently lacks state-of-the art modelling capabilities: 1) Energy system integration; 2) Spatial interdependencies in the energy system and spatial impacts of the energy transition; 3) Behavior and policy; 4) Impact of energy transition on economy and society. Evidently, we cannot fully address all these challenges within the ERP alone, as already noted above. Therefore, in the SEED-ERP we combined the results of an extensive review of the international literature, an inventory of existing energy (related) models at TNO, expert views of 25 TNO modelers and an energy modelling case study, to prioritize 4 modelling capabilities that we think TNO should invest in first and foremost. This prioritization is thus a key result of the SEED-ERP:

1) Big data (BD) & machine learning (ML): We need to fundamentally improve our energy systems models (notably TIAM-ECN and OPERA), with ML and BD techniques. To this aim we need to systematically analyze the dependencies of energy demand and energy supply on various drivers from large sets of empirical observations related to e.g. detailed geographical and climatological information.

2) Multi-scale and spatial modelling: We need to develop a language/method to combine models at different scale ('LEGO-isering' of models). In addition we need to invest in spatio-temporal modelling of supply and demand mismatches by using SOTA modelling techniques and computing capabilities including management of big-data sets. Finally, we need to overcome incorporate spatial modelling (resolution, granularly, uncertainty) in energy scenario development.

3) Behavioral modelling: We need to engage in different approaches developed in marketing and behavioral economics to quantify drivers & barriers of agent-based decisions and to subsequently implement behavior in existing energy system models.

4) Model linkages & digital twins: We need to invest in developing TNO's single market models (like gas or electricity models) into multi-commodity market models. Also, we need to better link optimization and simulation approaches and to better link energy system models with macroeconomic and mobility models.

These modelling capabilities use a combination of new insights from energy economics, spatial sciences and social sciences and also benefit from recent fundamental research results in energy systems and related modeling tools that make use of rapidly increasing computing power, AI and machine learning methods.

In addition to this agenda-setting, we performed a case study to develop a new integrated modelling framework based on a combination of optimization and simulation models to analyze the heat transition at a regional level. More specifically, we linked two existing TNO energy models – OPERA and ESSIM – and subsequently enrich the resulting modelling framework with CALLIOPE, a geospatial optimization modelling tool. We applied this modelling framework to the case of the heat transition in the province of Groningen in the Netherlands, to examine how we can convert geographically detailed data into a model on a higher scale. This is of course especially relevant for heat: both the demand and the supply (geo, residual heat) are very geographically determined and heat cannot be transported over long distances.

We succeeded in developing a working prototype of our integrated modelling framework. The main benefits of our new modelling framework are the following. First, because we take as a starting point a national model, certain assumptions do not have to be made beforehand. These assumption include, for example: what emission reduction should be assigned to the region of interest? What share of the national CCS potential can be allocated to the region of interest, et cetera. This means that using this combination, regions do have to be analyzed in isolation, which is often the case in regional analysis. Second, our approach exploits the strengths of both

optimization models and simulation models. Third, our approach allows to add information about the spatial aspects of certain energy system scenarios.

An improved and comprehensive energy modelling suite for policy support strengthens the TNO proposition in the energy domain, in mobility and transport and in circular economy and may serve as fundamental input for the establishment of a "Energy Transition Knowledge Center" (KCET) as joint initiative of TNO & EZK. Through its contribution to KCET, this SEED-ERP laid out a vision to strengthen collaboration with EZK, PBL, RVO, CBS, CPB.

The integrated modelling framework approach that we developed to analyze the heat transition in the province of Groningen bears the promise of policy relevance. Currently, regional analyses of energy system issues often consider a region in isolation. A good example is the so-called 'start analysis' by PBL, in which an inventory is made about the best options to realize natural gas free neighborhoods, for each municipality in the Netherlands. The approach taken analyzes all municipalities independently of each other while assuming that clean energy resources like hydrogen and green gas are always available at a given price. Obviously, the latter assumption is problematic because at a national scale the availability of green gas is very limited while a large increase in hydrogen demand will result in a price increase, potentially making hydrogen a less attractive source. These kind of effects can of course only be addressed if a regional analysis is embedded in a wider geographical context. Inclusion of these effects could give regional policy makers a much more realistic insight as to what is the optimal strategy to following in greening the regional energy system. The modelling framework that we develop in this project allows for an analysis of regional energy system requirements and constraints in interaction with the energy system at a higher geographical scale.

Realized contribution to the market position

As noted before, the ERP plan has not been awarded funding in the form of a Full ERP project, but currently serves as important strategic input for strengthening the Energy Transition research programming. Part of this is the setting up of an "Energy Transition Knowledge Center" (KCET) in collaboration with EZK. At the end of 2020, partly based on the results of the SEED-ERP project, we drafted a substantive proposal for the KCET that we will present in the near future to various stakeholders within and outside TNO.

The SEED-ERP led to a research agenda that is of strategic importance to TNO. We will use the results of this project, as summarized in the ERP plan, as a starting point for participating in external funding opportunities. This includes NWO calls, like for example the 'Vraaggedreven Partnerschappen voor Consortia'.

In developing new modelling tools we aim to follow the current demand for Open Source software.

Publicity

Publications

- Boonman, H., Mulder, P., *Short Description of TNO's Energy Models*, TNO report ??, 2021.
- Boonman, H., Faaij, A., Mulder, P., *ERP Plan for New Generation Modelling suite for Informed Energy System Transitions*, Unpublished paper, 2020.
- Matthijssen, E., Mulder, P., van Straalen, J., Westerga, R., *Spatial modelling of heat transition. The case of Groningen*, TNO-rapport, 2021.