TNO EARLY RESEARCH PROGRAM
Annual Plan 2021

2020 S 083

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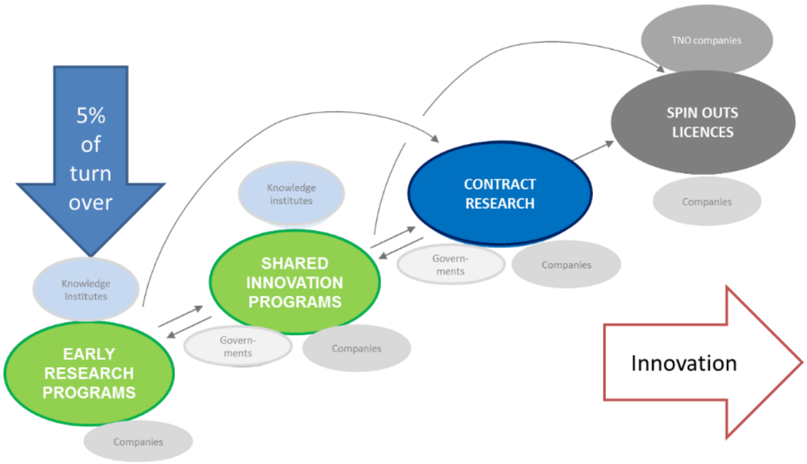
Contents

Introduction

The Early Research Programs (ERP's) presented here reflect TNO's vision where to put its innovative research efforts to be able to grow strong technology positions and to contribute, together with knowledge partners and stakeholders, to societal challenges and economic impact. These programs are meant to build, renew and maintain TNO's knowledge assets ('Kennis als Vermogen'). The ERP's represent about 5% of TNO's turnover. The remaining 95% is steered by TNO's stakeholders: clients, 'Topsectors' and Ministries (via consultation) and MOD, EZK and SZW (via task financing).



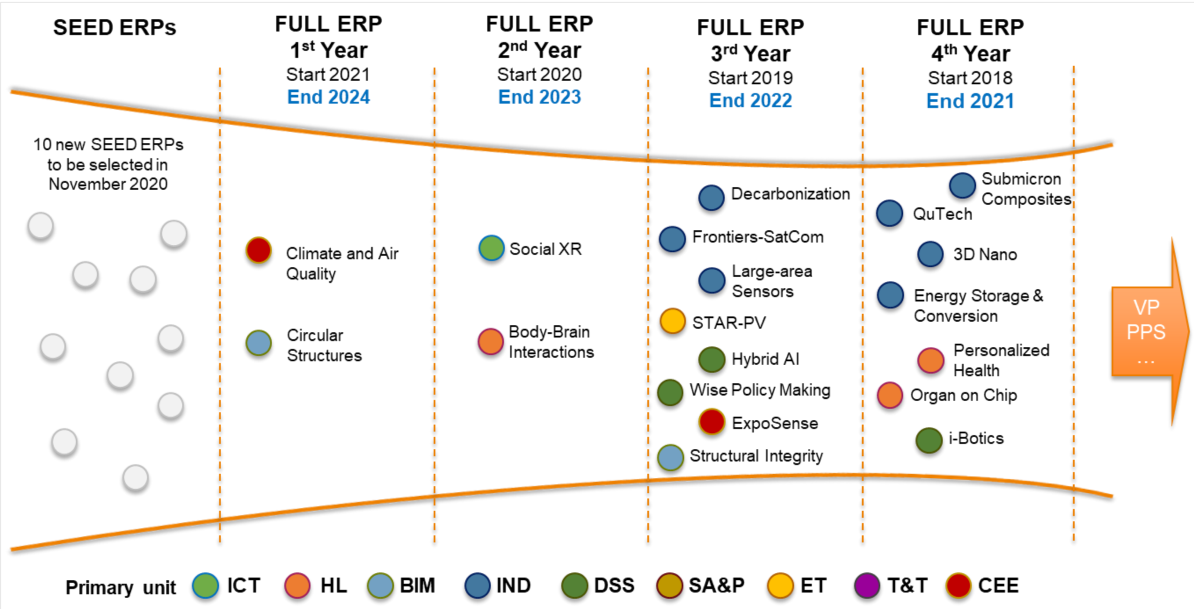
The main characteristics of the ERP portfolio are as follows:

- The programs build and renew strong technology positions in the focus areas defined in the TNO Strategy Plan 2018-2021
- The programs are use-case inspired and have clear research goals: ERPs feed multiple innovation roadmaps of TNO, often from different units with common requirements for lower-TRL technology breakthroughs. The output of the ERPs is transferred to (higher TRL) shared innovation programs and contract research.
- The programs aim for added mass through collaboration with knowledge partners such as universities and additional co-investments by stakeholders.
- The programs have substantial mass (usually > 1 mln Euro ERP budget per program) and have a typical duration of four years.
- ERP funnel management (involving reviews by TNO Corporate Science Office and by the board of TNO's Science Directors) is in place to monitor the progress and to adjust and reallocate resources if necessary.
- Together with EZK we inform the Topsectors and Ministries of our approach of building our knowledge base via the ERP's, aiming at early involvement of companies and other stakeholders in public private cooperation.
- 'Full ERP' programs are usually preceded by one-year 'Seed ERP' projects that explore the feasibility of the topic, substantiate the impact to be expected and build required partnerships, thus developing the full ERP program. Out of the six 'Seed ERP' projects 2020, the two strongest were selected for continuation as Full ERPs in 2021 and onwards.

The ERP portfolio includes a large number of programs initiated in 2018 and 2019 (see figure below). An important goal of the ERP portfolio management is to bring the portfolio to a 'steady state' in which every year a similar number of existing ERP's (4-5) ends and new ERP's can be initiated. Only then will TNO be able to respond with agility to new technology trends and needs and will TNO's researchers be stimulated to continuously be on the outlook for impactful new research directions, knowing that there is an instrument to award and adopt the best ideas. For 2020 and now also for 2021 some budget has been freed from the large set of ERP's started in

2018 and 2019 to at least initiate two new ERP's yearly. Moreover, one ERP (Self-adapting Smart Batteries) has been terminated (as ERP) before the end of its four-year term as sufficient technology maturity had already been reached to proceed outside the ERP portfolio. The two new ERP's to start in 2021 concern 'Climate and Air Quality' and 'Circular Structures', both being domains with clear scientific challenges and high societal relevance. These two topics were selected out of the six 'Seed ERP' topics of 2020. As of 2022 we will be able to fully implement the intended 'steady state' approach for portfolio renewal. Anticipating this, we will increase the number of Seed ERP's to be executed in 2021 to 10. We feel that a success rate of about 50% for Seed ERP's to be promoted to Full ERP's is a healthy target.

ERP Funnel 2021



In the following chapters of this report each of the ERP's is described by its overall goals and its intended results in 2021. Each chapter consists of paragraphs describing (1) the problem addressed, (2) the positioning of TNO with regard to this topic, (3) the overall program objectives and approach, (4) the partnership and applications and (5) the concrete results targeted in 2021. The first three paragraphs are more or less 'constants' over the program duration, whereas the paragraphs regarding intended results 2021 against achieved results 2020 provide the 'actuality'. The table below provides the ERP summary, listing the ERP titles and a selection of the most prominent targeted results in 2021.

ERP	Planned results 2021
Quantum Computer / Internet	Requirements definition for a NISQ (Noisy Intermediate Scale Quantum) computer (in a NISQ computer the error correction needed to reach fault tolerance is not yet included, but the system allows to tackle problems in a way that cannot be done by classical computing); upgrade of Quantum Inspire (Europe's first full-stack prototype platform for quantum computation in the cloud) with a second two-qubit chip; demonstration of long-distance entanglement between Delft and The Hague (towards 'Quantum Internet');
Energy Storage & Conversion	Photons-to-chemicals: a lab-scale mini-factory operational for CH4 production and an economic feasibility study of te technology published. Electrons-to-chemicals: a proof-of-concept of integrating CO_2 capture from simulated flue gas with conversion; a proof-of-principle of integrating CO capture with electrochemical conversion into C2 molecules.
3D Nano Instruments	Sub-surface Scanning Probe Microscope with improved performance (optimal signal-to-noise ratio, cantilever tip roughness and tip smoothness to

	increase performance and reproducibility by 25%), needed for 'overlay measurement' on next-generation chips. Measuring material/ chemical composition at nano-scale: demonstration of application-relevant performance (10nm resolution on a sidewall and/or in a confined space). Quantum sensing: evaluation of the proof-of-principle instrument developed in 2020 on certain types of memory chips (e.g. high density STT-MRAM or MTJ Pillars).
Digital Twin for Structural Integrity	Toolkit (enabled by exascale computing) to compose digital twins of bridges. With such digital versions of bridges we can explore optimal sensor type and placement and the type of anomaly signal in case of deterioration. Table-top demo (with Bundesanstalt für Materialforschung und -prüfung) of a digital twin of a bridge showing real time system identification and damage detection.
Personalised Health	'Human proof of concept study': real-life test of the integration of technologies and knowledge that have been developed during the first three years of this ERP. Aim is to show that a 'personalised combined lifestyle intervention' stimulates a healthy lifestyle and can reduce low-grade inflammation in people with overweight and/or obesity who are cardio-metabolically compromised.
Organ on Chip	Gut-on-chip: a proof of concepts of stem-cell based cultures on a chip and gut organoids on a chip. Liver-on-chip: a validated co-culture model for a specific liver disease (NASH); demonstration of effects of combination drug therapies.
Submicron Composites	Sustainable buildings: an A4-sized demonstrator of an energy efficient window with pigmented PVB film as thermochromic interlayer. Additive Manufacturing: material and processing strategies to 3D print fiber-reinforced parts with thermal properties (i.e. thermal stability > 125°C) suitable for high performance (aerospace) applications.
i-Botics	Method/model for visual scene understanding in a robotic context, with a large variety of perceived objects using a hybrid AI approach. Demonstrator of an 'active back support' exoskeleton; smart, mobile calibration of such an exoskeleton.
Hybrid AI	SNOW (Safe autonomous systems in an open world): improved real-time hybrid AI software for a quadruped robot (requiring two times fewer operator interventions in the search and rescue experiment than in 2020). FATE (Responsible human-machine teaming in a dynamic world): comparison of possibilities and limitations of bias-controlling measures; scalability studies for secure federated learning.
ExpoSense	Miniaturization of TNO's portable IR-spectroscopy-based solution for chemical identification making it wearable, with target costs of less than 2000 EUR. Demonstration in city of Eindhoven of our capability to estimate and predict the personal exposure of individuals to particulate matter based on their GPS tracks.
Frontiers-Satcom	System concept for a 10 Terabit/s ground-to-satellite feeder link with 30 times higher data rate. System concept for a multi-beam communication terminal at a GEO satellite, reducing swap by factor 3. Dynamic tracking system for aircraft links, allowing for up to 100 parallel targets.
Wise Policy Making	A web-based prototype (TRL 5) that includes 1) a library of wellbeing models, 2) functionality to collect, analyze and visualize wellbeing data and 3) dashboard to support the policy makers' evaluation of the effects on wellbeing.
Sustainability & Reliability for PV	Design concepts for mechanisms reducing the sensitivity of CIGS PV (photo voltaic panels) to partial shading; test modules of PV with integrated sensors for combined stress monitoring (T, stress, humidity), installed at TNO field labs for Building-integrated PV and floating PV; a TNO research agenda for recyclability and eco-design of Building-integrated PV.

Body-Brain Interactions	Analytical platforms bridging preclinical and human platforms (e.g. plasma biomarkers; readouts for stressors; functional MRI imaging of brain); Plasma profiling to identify microbiota-derived metabolites and lipids, proteins, metabolites that mediate effects gut -> brain; adipose -> brain and liver -> brain interactions.
Social eXtended Reality	Proof of concept of automated spatial calibration and synchronization of visual and tactile data from multiple users in a shared eXtended Reality environment.
Large Area Ultrasound	Real-time ultrasound imaging array with portable readout electronics: enabling to do application-specific tests outside the acoustic lab. Demonstration of a concept for channel reduction: addressing millions of elements while keeping the number of input-output channels low (100-200) using novel 'channel reduction' schemes.
Decarbonisation	Plasma technology for CO2-free simultaneous production of hydrogen and ethylene: first design of a prototype reactor (TRL 2-3). Recycling polymer and household waste: options for controlling the product formation in the Milena/Olga gasification process. Feasibility study on the possibilities to obtain a new "green" grade of pyrolysis oils by partial dissolution of plastic waste in naphtha-like media.
Climate and Air Quality	Static high-resolution (25m) annual base emission map for the Eindhoven area based on existing information from the national emission inventory combined with spatial proxies. Benchmark indicator set for the TNO open-source model LOTOS-EUROS (1x1km) for particulate matter, greenhouse gases, nitrogen.
Circular Structures	Methods and prototype to determine the critical dosages for blending of (in)organic additives with construction and demolition waste (CDW) needed for disclosing the CDW's maximum potential and for enabling increased cement replacement levels higher than 50% (state-of-the-art is at 10%).

To illustrate how the ERP relate to the TNO strategic areas as laid down in the TNO Strategy 2018-2021, the table below is provided.

ERP	Nano & Quantum	Hybrid energy systems	Smart and green materials	Smart megastructures	Media synchronisation	Artificial Intelligence	Robotics	Neurotech / Medtech	Subsurface Engineering (Geology)	Valorisation of (meta) data	Inside the Human Body	Inside the Human Mind	Integr. social-system modelling and forecasting	Security (ICT)
	STRATEGIC AREAS 2018 - 2021													NEW
Quantum Comp	X													X
3D Nano	X							X						
Optic Sat Comm	X						X							X
Large Area Sensors	X		X					X			X			
Sust. & Reliab. PV	X	X	X											
Energy Stor & Conv		X	X											
Subm composits		X	X				X							
Structural Integrity				X										
Hybrid AI						X				X				
i-Botics							X					X		
Organ on Chip											X			
Personalised Health											X			
Exposense	X		X								X			
Wise Policy Making												X	X	
Decarbonisation		X	X										X	
Body brain interaction											X	X		
Social XR					X									
Climate and Air Quality										X				
Circular Structures			X	X										

Quantum Computer and Quantum Internet

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

Program description

QuTech is a mission-driven organization, focused at building scalable prototypes for Quantum Computing and Quantum Internet. QuTech is founded by TU Delft and TNO and coordinates the research and engineering on Quantum Computing and Quantum Internet for both organizations. ERP is an integral part of the 10-year base funding that TNO, TU Delft and other covenant parties allocate to QuTech.

The first phase of QuTech (2014 – 2017; Proof of Principle) focused on accelerating research and making the transition towards a mission-based way of working. The current phase (2018 – 2022; Proof of Concept) is used to demonstrate progress on key technologies (critical milestones) resulting in the following QuTech deliverables in 2022:

A. An online platform giving access to a pre-prototype fault tolerant quantum computer based on three qubit technologies that currently are being considered scalable: superconducting qubits, electron spin qubits and spin qubits in NV centers.

B. A pre-prototype quantum internet consisting of a three-node internet between The Hague, Delft and a third node of which the location still needs to be determined accessible through an online portal allowing quantum communication between nodes.

Both pre-prototype deliverables (demonstrators) play a key role in bringing this new technology to society. In order to do so, an ecosystem is being created to increase our connectivity with stakeholders. TNO's role is to do applied research, increase TRL of the Quantum Computer and Internet systems and bring QuTech technology to society.

Next to the demonstrator projects, support projects are executed in the ERP program. Support projects focus on strengthening the research projects executed in QuTech under the responsibility of the QuTech Principal Investigators (group leads and professors), with the research and engineering strengths from TNO.

1. Problem definition

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. Due to recent breakthroughs in for instance nanofabrication, cryogenic technology and high-frequency electronics 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 Quantum Communication which is inherently safe from eavesdropping.

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 by multi million euro investments by companies (Intel, Microsoft, IBM, Google) and nations (Netherlands, USA, China, UK). The European parliament chose quantum technologies as the third (and so far final) Flagship with a 1 billion budget over 1 10-year run-time. Within The Netherlands, the National Agenda Quantum Technology underlines the societal and economic relevance of quantum technology.

2. Positioning

In this challenging environment TNO is well positioned due to the partnership with TU Delft called QuTech and the intense cooperation with Microsoft and Intel. The combination with TU Delft in the QuTech organization offers a unique environment to combine the necessary world-class research and exceptional engineering that is required to deliver full stack quantum systems. The recent launch of the first online quantum computing system in Europe, Quantum Inspire, is a clear success of this unique cooperation. The system also holds the first online (accessible) spin qubit system in the world. The recent launch of the NetSquid simulator has followed. The QuTech organization uses roadmaps to further advance the research. ERP funding is a key building block in these roadmaps.

Recent developments include a strong development of the Delft ecosystem, and an increase of spinouts and new industrial partners. Due to the technology involved as well as the relevant industrial players, i.e., potential customers of TNO, quantum technologies are positioned as an extension to TNO Unit Industry's Semicon Roadmap. Nanofabrication for quantum computing, for example, generates new knowledge that could also be relevant to TNO's existing partners in the semiconductor industry. Quantum-based applications create new opportunities in the combination of quantum hardware with quantum algorithms in TNO-ICT.

3. Objectives and approach

Organizational objectives

Driven by the objectives of QuTech and the need for a tighter integration of research and engineering, QuTech will be re-organized into three divisions (along the research lines as defined below). Each division will be managed by a division research lead (DRL) from the TU Delft and a division engineering lead (DEL) from TNO, in accordance with the new QuTech governance, also in line with the recommendations of the mid-term review by the Dijkgraaf committee. The introduction of the new governance will increase the strength of the cooperation towards the QuTech mission.

The overall multi-year objective of the program - to develop a prototype quantum computer and a multi-node prototype quantum internet – will remain the same: a joint effort from both partners forming QuTech.

ERP Research Line A "Quantum Computing"

The original objective for this research line was to develop a prototype fault tolerant quantum computer: *The Fault-Tolerant Quantum Computing roadmap aims for a full-stack scalable quantum computing system, including the qubit circuits, the control electronics, and the software layers such as compilers. The approach to achieve fault tolerance is based on quantum error correction, in which information is encoded redundantly enabling error detection without destroying quantum data. The qubit hardware systems are electron spins in quantum dots and superconducting quantum circuits.*

This goal still remains, but will be refined. Up to this year the focus of QuTech was on the development of a Fault Tolerant quantum computer with error correction. Although this is still seen as the holy grail of quantum computing, the level of maturity that is required will probably not be reached in 5 to 10 years. Therefore, the power of quantum computers must also be used in a different way, formulated as NISQ computer (Noisy Intermediate Scale Quantum computer). In a NISQ computer the error correction that is needed to reach fault tolerance is not included, but the system allows more flexibility and other ways to increase robustness to tackle problems in a way that cannot be done classically. NISQ machines require another paradigm of programming and control. The main difference is the user interaction and the amount of user interference with the machine (which is higher and more complex than with fault tolerant machines) and the diversity of control signals (variations) which is increased. In 2021 we will start with determining the full requirements for NISQ machines, in interaction with potential users of such systems.

ERP Research Line B "Quantum Internet"

The goal of this research line is to build an optically-connected network of many (small) quantum computers. Such a network enables the exchange of quantum bits between any of the connected quantum processors in order to solve problems that are intractable classically.

A quantum network in which the processors are located at different geographical locations is called a Quantum Internet. Our goal is to develop the technology to enable quantum communication between any two places on earth. One application of such a quantum internet is to provide a fundamentally secure way of communication in which privacy is guaranteed by the laws of physics.

Quantum processors can also be connected into a quantum network in order to assemble a large quantum computing cluster. This approach is called networked quantum computing and offers a natural path towards scalability. Combining a quantum internet and a networked quantum computer finally allows remote users/providers to perform secure quantum computing "in the cloud".

ERP Research Line C "Qubit research"

The focus of the Topological Quantum Computing roadmap is to develop, build and demonstrate the first topologically protected quantum bit based on Majorana-bound states. We continued our efforts in combining material science, theory, and novel device design to obtain more control of the underlying constituents of the topological qubit. The so-called zero state- or Majorana qubits have the potential of very long coherence times.

4. Applications and partnerships

QuTech is a partnership between TNO and TU Delft and it is located at TU Delft directly connected to the TNO-STW location. QuTech uses mixed teams, facilitating a seamless way of working. The world-class scientific heritage of the TU Delft forms the foundation for QuTech. The total investment from TU Delft in the QuTech collaboration encompasses more than 150 fte scientific personnel (including PhD's and post docs), technical and support staff. Other financial partners in the QuTech cooperation include EZK and TKI (through TNO) and NWO (through TU Delft).

Strong scientific partnerships have been built up with Leiden University, SurfSara and QuSoft in various programs and in the National Agenda for Quantum Technology. There are cooperations with various RTO's in different programs, including EU, such as CEA-Leti and Fraunhofer.

QuTech works together with Microsoft and Intel. These companies contribute large amounts of money, as well as expertise. The activities within QuTech related Microsoft and Intel are defined in dedicated projects.

A growing number of partners is engaged in industrial projects, for instance Keysight, Zürich Instruments, KPN, and OPNT. Various spinouts have formed, such as QBlox and OQS, who start developing projects and opportunities with QuTech and more specifically with the TNO-part in QuTech.

TNO and TU Delft are participating in the European Flagship on quantum technology. The joint European institutes have a worldwide leading position in fundamental research in quantum computing. The solid state technology in Delft, the optical technology of the German speaking region, and the more fundamental research in England, France, and Denmark are complementary and together ahead of any other region in the world. QuTech, with the highest ambition towards industrialization of quantum technology is leading the initiative of developing a Quantum Internet blueprint in the QIA project of 10 MEuro with the majority of relevant European institutes and universities participating.

At the moment of writing this ERP plan, the contract negotiations of a 15 MEuro H2020 project called QLSI (Quantum Large Scale Integration) are being finalized. TNO acts as one of the WP leaders for this project, responsible for the upgrade of the Spin-2 setup (2 qubits) in Quantum Inspire to a 10-qubit setup (Spin-10) within the next 4 years. The consortium consists of 17 leading European academic, RTO and industrial partners on Si Spin qubit development and integration. A 22,5 MEuro Impulse from the National Agenda Quantum Technology has been allocated and its implementation is being finalized in 2020, leading to a considerable additional funding stream for the demonstrators and the ecosystem from 2021 onwards. The full National Agenda Quantum technology (more than 600 MEuro) has been submitted.

In parallel TNO and TU Delft will submit proposals to regular calls of H2020 and NWO. Some upcoming calls in H2020 open opportunities for funding of research and development in the field of quantum computing, quantum communication, or quantum technology in general. Some technological developments may also find funding by calls related to, e.g., low temperature electronics or integration of new materials into the process flows of More Moore. TNO and TU Delft are continuously involved in the discussion in shaping the calls and identifying which proposals will be submitted to which calls in the coming years. These activities are aligned with the overall multi-year objectives of the institute.

Plan Year 2021

Organization

Within the QuTech ERP we have *support projects* in three research lines and *demonstrator projects* in two research lines, which are partly covered by ERP funds and VP Semicon funds and partly by other funds. The 2021 plans for all projects (support projects and demonstrators) will be defined in October 2020, with a final decision made by the QuTech Board of Directors on 1 Nov. This means that the planning and approval process is out of sync with the ERP process at TNO. Aligning these processes is currently being done by the QuTech BoD and TNO.

For the three research lines combined there is roughly 3 MEuro budget for support projects, partly covered by ERP. The allocation division per research line is based on the number of PI's in that research line. The research topics were defined by the roadmap leaders of FTQC (Fault Tolerant Quantum Computing), QINC (Quantum Internet and Networked Communication) and TOPO (Topological Quantum Computing), together with the PI's and with approval by the SD (Shared Development) roadmap leader. In the new organizational structure, the prioritization will be done by the Division Research lead (DRL) with input from the Division Engineering Lead (DEL). The topics are not known yet. They will be prioritized towards the QuTech mission.

For the demonstrator projects combined there is roughly 2 MEuro budget, partly covered by ERP. Budget allocation is done by the QuTech BoD based on the project proposals made in October. The overall strategy for the demonstrators is set in consensus by the DEL, DRL and Director Business Development. Although the exact plans for the demonstrator projects need to be agreed on by the QuTech board, below we will give a rough outlook for the 2021 plans for the demonstrator projects.

A. Plan – Research Line "Quantum Computing"

A.1 Key results so far

In line with the projected goals, we officially launched Quantum Inspire (QI) in April 2020, which is:

- Europe's first full-stack prototype platform for quantum computation in the cloud.
- The world's first spin-based quantum processor in the cloud.
- The world's first quantum computer in the cloud supporting multiple qubit technologies.

QI is a platform with a high degree of modularity and offers the public cloud-based access to two programmable quantum processors:

- (1) SPIN-2: a 2-qubit processor based on spin qubits in Silicon, and
- (2) STARMON-5: a 5-qubit processor based on superconducting transmon qubits.
- Earlier developed automated tuning and calibration algorithms have been incorporated in QI

On the support side, TNO delivered the Central Controller, a key element in the coordination of qubit control signals in the Starmon-5 setup. Furthermore progress was made on the wafer growth and quantum dot fabrication.

A.2 Key objectives and expected results

- Upgrade Quantum Inspire with a second two-qubit Si electron spin chip (silver device) with its own electronics. This chip serves three key objectives
    - Serve as an R&D tool to test upgraded hardware and software components
    - Backup for the first electron chip (golden device)
    - First step towards a 4-qubit electron chip and 10-qubit electron spin chip in the next 2 to 4 years
- Delivery of IQ-UPC. IQ-UPC is an integrated IQ modulator and Upconverter for MW frequencies between 1 and 20 GHz. The IQ UPC is meant to generate the control signals for both Transmon qubits, electron spin qubits and NV centers and can thereby serve multiple qubit technologies. The functionality and performance of the IQ UPC for qubit control matches that of standard COTS equipment which is 10x more expensive and which also has a much larger footprint. First conversations for IP transfer/licensing are ongoing.
- Improvement of automated tuning and calibration both for electron spin qubits and transmon qubits.
- In 2021, we will see the start of the funding for the National Agenda Quantum Technology. In this 7-year program the goal is to further develop our quantum computing efforts and integrate it in a national program that aims at upscaling the amount of qubits and growing the ecosystem. Part of this effort is the development of a NISQ quantum computer. In 2021 we will begin with formulating the requirements for this system
- Also in 2021, the H2020 QLSI project will start, matched with QuTech funds, with a goal for 2021 to prepare the QI set-up for a system of 10 electron spin qubits.

B. Plan – Research Line "Quantum Internet"

B.1 Key results so far:

- Frequency conversion system long term stability achieved (optical alignment and conversion efficiency)
    - Total conversion efficiency of 12…16% reached and maintained 24/7
- Frequency locking of (laser) nodes to the mid-points while allowing single-photon transmission (key requirement for system)
- Software infrastructure (QMI) for executing distant multiple node entanglement generation
- Netsquid (part of QIA project, matched with QuTech ERP) has been released

B.2 Key objectives and expected results

- Long-distance entanglement generation between Delft and The Hague (using the key components that were developed up to now).
- Optical phase stabilization of the Qlink system.
- Start of the assembly and integration of a 3rd node besides Delft and The Hague

C. Plan – Research Line "Qubit Research" (Topo roadmap)

Key results obtained this year were the creation of 2D nanodevices and software development on Kwant. In this research line TNO does not execute any demonstrator projects, only support projects. The contents of these projects will be defined later this year.

Energy Storage and Conversion

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

Program description

1. Problem definition

In the last decades, the massive use of fossil fuels had a big impact on the emission of CO_2. A strong acceleration is needed to timely transform the Dutch energy landscape from the current fossil fuel based one to a CO_2 neutral renewable energy infrastructure based on the goals as set by COP21 and 22 (UNFCCC), and accorded by the EU (RED) and the "Energie agenda". Conversion and storage of renewable energy are pivotal for achieving this change. In the next 20-30 years, the way how energy is generated, stored, supplied, priced and sold will be fundamentally different from the current approach. A key step in the transformation to a renewable energy infrastructure is the conversion of renewable energy sources such as solar and wind into usable energy forms such as electricity. Due to the intermittent nature of these renewable energy sources, however, there is a strong need to store energy on a large scale in a cost efficient manner. Based on its high storage density, rather low cost, flexibility in use for various applications, and ability of use in the current infrastructure, conversion of renewable energy to fuels would be an ideal solution. It is to be expected that significant amounts of fuels are needed for e.g. the heavy transport sector and the chemical industry.

The chemical industry is in principal well suited to use electrical energy for their primary and secondary processes, and is therefore one of the sectors that can also contribute to the Netherlands government goals as stated in the "Energy Agreement for Sustainable Growth". One of the objectives of this agreement is to increase in the portion of energy generated from renewable sources from 4.4% (2013) to 14% in 2020 and to 16% in 2023. It is of importance to note that the Dutch chemical industry is under pressure, it is facing enormous economic and ecological challenges in the next decades. Increased global competition, geographical shifts in demand and high price volatility of products and feedstock ask for a more flexible and efficient use of employed capital (production plants) and resources (personnel, energy, raw materials). Recently, it has become clear that the European chemical industry has to drastically accelerate its innovation process to stay in business. To reverse this trend and reinforce the global competitiveness of our industry the Topsector Chemical Industry in The Netherlands has formulated a strategy based on two main topics:

- Strengthen the current clusters that are primarily focused on bulk chemical production.
- Within these clusters, stimulate the generation of more high added value products targeted at new applications of chemicals and replacing less sustainable chemicals by green chemistry.

In the ERP Energy Storage and Conversion we focus on the use of renewable energy, i.e. renewable electricity and sunlight, CO_2 and green H_2 as a feedstock to produce the C1 chemicals and fuels CO, HCOOH (formic acid), CH_3OH (methanol) and CH_4 (methane), which provides 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. It changes the actual energetic system towards a sustainable system and simultaneously implements a CO_2 neutral system.

2. Positioning

Research Line "Photons-to-chemicals"

The exploration of new solar energy harvesting technologies has attracted much interest. One of these new approaches is the direct use of sunlight to power chemical processes. More specifically, the absorption of light by catalytically active metal nanoparticles, viz. plasmon catalysis, is used as a way to capture solar energy and use it for the production of molecules with added value. This concept facilitates a much higher photon-to-product efficiency than conventional semiconductor catalysts - up to 56% vs. <<1% - which translates into a 10^4 x higher space-time-yield, 10^4 x less land use and a techno-economically much more favorable process concept. Upon irradiation with visible light, through the localized surface plasmon resonance (LSPR) effect of plasmonic nanoparticles, plasmon excitation occurs, followed by two competing plasmon decay pathways. One is the radiative process, which is dominant for metal (e.g. Au) NPs that are larger than 40 nm, where the plasmon quantum decays into a photon. The second pathway, which is dominant for small NPs (< 40 nm), is a nonradiative process, where a free electron of the plasmonic NP is excited into a higher energy level. Such "hot" electrons may decay in two ways. Firstly, a rise in the lattice temperature of the metal nanocrystal may result. This thermal energy is thereafter dissipated to the surrounding medium, leading to plasmonic photothermal heating, which may accelerate chemical reactions. Secondly, if an electron acceptor is present, the hot electrons may transfer into its electronic states. Direct interactions between plasmonic NPs and reactive molecules has been reported, which involve direct injection of the excited hot electrons from the NPs into the lowest unoccupied molecular orbital (LUMO) of adsorbed molecules. The occupation of the antibonding orbitals will weaken the related bonds, induce bond dissociation and initiate chemical reactions. This effect is called *plasmonic photocatalysis* and leads to the direct harvesting of solar energy for desired chemical reactions such as hydrogenation of CO_2 to C1-chemicals and fuels.

Thus far, a limited number of cases of plasmonic photocatalysis have been reported in scientific literature, such as dissociation of H_2 on Au, oxidation of alcohols, reduction reactions, imine and amine synthesis, hydroxylation of phenol, synthesis of propargyl amines, and Pd-catalyzed cross-coupling reactions such as the Suzuki reaction. In many of these cases, the observed rate enhancements are ascribed to a combination of two effects: firstly, plasmonic photocatalysis through the injection of hot electrons into LUMO orbitals and secondly, plasmonic heating leading to photothermal conversion. In many cases, plasmonic photocatalysts suffer from poor stability, which is overcome by using metal oxides as support materials. The support material is observed to play a large role on the activity of these systems. CO_2 hydrogenation has been considered a way to generate green fuels and close the carbon cycle. In the last years photo-assisted plasmon catalysis has been studied to produce CH_4 from CO_2. In 2019 TNO published the results of the ERP, where Ru nanorods were studied under solar light illumination to produce selectively methane. We identified large nonthermal contribution when the catalyst was irradiated under slightly concentrated solar light irradiation of 5.7 and 8.5 sun intensity. The photon-to-methane efficiency of this plasmonic catalyst is 55% that is one of the best reported in the literature. The reverse water-gas shift (rWGS) reaction is an interesting second reaction we are developing to produce CO from CO_2 and renewable H_2 with sunlight as the energy source. The resulting CO product can be used to synthetize methanol, or higher hydrocarbons via the well stablished technology of Fischer-Tropsch. In 2019, we a started the design of a tailored reactor for plasmon catalytic conversions. This is required to establish a demonstrator that enables technoeconomic validation. This development was continued in 2020, first designs of a mini-factory were made together with partners. The fabrication of the mini-factory will be established and validated for CH_4 production in 2021. In 2019, we have developed initial concepts for photochemical and photoelectrochemical water splitting for producing green hydrogen. This is selected based on business case studies for hydrogenation of CO2 that clearly illustrate that the high costs for green hydrogen from electrolysis negatively impact the business case. The results of this study resulted in a new seed-ERP entitled 'Solar to Hydrogen'. In 2020 we have further expanded the research with the development of strategies of commercially feasible photo(electro)chemical conversion of CO_2 to methanol. Knowledge and technology has been acquainted on new and unique technology for chemical energy storage, synthesis and structural, compositional, optical characterization of metal containing nanoparticles, scale-up of metal nanoparticles materials used as catalyst, infrastructure for determination of conversion and yield in nanocatalysis using metal nanoparticles, with closed mass balances, converting sunlight directly into chemical energy using nanoparticles as catalysts, development of photoreactors, establishing protocols for CO_2 photoreduction in different solar fuels (e.g. methane) and harvesting sunlight and reducing CO_2 to produce solar fuels, and economic studies on sunlight powered chemical processes.

Research line "Electrons-to-chemicals"

In the past period, the ERP has created an active internal research group with electrochemical expertise and infrastructure, and on the other hand strengthened the external network with academia and companies primarily interested in CO_2 valorization using electrochemical conversion technology. TNO strategy regarding electrochemical conversion is to be worldwide leading regarding scaling up of electrochemical processes from lab to pilot and industrial scale, and particularly for specialty and commodity chemicals (starting from CO_2). Significant knowledge and infrastructure steps have been made specifically focussed on electrosynthesis, electrode and process development. Outside TNO, in the Netherlands, the field of electrochemistry is growing mostly in academia. TNO has joined several universities in active projects aiming at electrochemical conversion such as the Elerecet (CO_2 to ethylene, via NWO) and E-Triple-C (CO_2 to CO, via ISPT) project. This places TNO in a strategic position to evaluate the progress that academia is making in this field. In the next years, the network created is being strengthened by the creation of new collaboration projects involving TNO, academia and companies. Also the collaboration with companies has been strengthened. The results obtained in ERP of the previous years have led to the creation of the E-COUCH project (paired electrolysis CO_2 to CO and HCl to Cl_2, via TKI) , the PHECAM project (CO_2 to formic acid, via TKI), and the E2C project (CO_2 to formic acid in a pilot installation of a capacity of 1kg/h, via Interreg, started already in 2018).

Especially in academia significant research efforts have been directed towards the electrochemical conversion of CO_2. These efforts have been mainly targeted towards optimization of the electrocatalyst (i.e. improving selectivity and current density), and towards finding new suitable catalyst materials for selective CO_2 reduction processes. TNO has a strong Dutch network of academic partners allowing identification of possible suitable novel electrocatalysts. In addition, the majority of these academic studies are performed in laboratory scale batch reactors and are far from industrial applications. Little amount of work has been done on electrochemical engineering aspects and even less on system development. However, in the past years the CO_2 electrochemical reduction field is moving towards the development of semi-continuous processes in flow reactors. Special attention is now paid to the development of gas diffusion electrodes in order to overcome the limitations of CO_2 electroreduction which leads to low energy efficiencies. However, these studies are still far from industrial scale since low current densities (<300 mA/cm^2) are often reported and durability and stability tests are not addressed. TNO's approach is the development and scale-up of the overall CO_2 electroreduction system towards an industrially relevant scale paying special attention to system integration, particularly the integration of CO_2 capture and electrochemical conversion.

3. Objectives and approach

Energy conversion and storage becomes increasingly important to realize the vital transition from fossil fuels to sustainable energy. In this program we focus on searching for new techno-economically feasible chemical storage processes, resulting e.g. in the development and validation of plasmonic catalysts to reduce CO_2 to CH_4 using sunlight as energy source, and the development of a process and reactor concept for the reduction of CO_2 to HCOOH using renewable electricity as energy source. We strongly collaborate with industry (e.g. via VoltaChem and the Brightlands Chemelot Campus and Site), academia (e.g. Utrecht University (via professor Weckhuysen multiple master students for internships), Leiden University, Delft University, Hasselt University (professorship Pascal Buskens, PhD student Daria Burova, postdoc Ken Elen and joint postdoc with Antwerp University), Zuyd University of Applied Sciences (subcontracting Tim den Hartog, multiple bachelor students as interns) and Forschungszentrum Jülich, Deutsches Zentrum für Luft- und Raumfahrt, ETH Zürich, EPFL Lausanne, Fraunhofer ISC via EU project proposals), and national and regional governments.

Our focus is on the development and validation of concepts and processes at a technology readiness level of 2-4 that use electricity from renewable sources (solar, wind) or sunlight directly to convert CO_2 to C1 chemicals and fuels CO, HCOOH, CH_3OH and CH_4. For both chemicals and fuels, the ultimate goal is to provide technologies and concepts that can be scaled up to an efficient production process at a cost which will be competitive with their fossil-based analogues in the period 2030-2050.

To date, we have identified two attractive routes towards hydrocarbon based fuels. These two routes are interconnected. The first route (indirect) is based on generation of renewable hydrogen, and the subsequent reaction of this hydrogen with CO_2 towards hydrocarbons. The second route (direct) is based on the direct conversion of CO_2 and water towards hydrocarbons. The technologies related to these routes are based on electrochemistry and on photochemistry.

The research line Photons-to-chemicals is focused on the conversion of CO2 to C1 chemicals and fuels CO, CH4 and CH3OH, using sunlight as energy source for driving the reaction. The long term goals are:

- To develop and validate efficient catalysts for production of the C1 chemicals and fuels CH4, CO and CH3OH through sunlight-fueled hydrogenation of CO2 with high space-time-yield, minimized CAPEX and land use.
- To develop suited reactors for sunlight-fueled chemical processes, and combining these with catalysts and additional components to realize a lab scale mini-factory (TRL 4-5).
- To develop catalysts for production of C>2 chemicals, e.g. ethylene or ethanol, through reductive coupling of CO2

The research line Electrons-to-chemicals is focused on the process development for the conversion of CO2 to C1 chemicals and fuels, e.g. 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 CO2 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/m2;
2. Faradaic efficiency should be above 50%;
3. Power consumption lower than 500 kWh/kmol;
4. Electrode lifetime should be above 8000 hrs.

The ERP Energy Storage and Conversion has established strong strategic partnerships with key academic (e.g. Prof. Weckhuysen/Utrecht University, Prof. Koper/Leiden University, Prof. Mul/Twente University, Prof. Van Bael & Buskens, PhD student Daria Burova, postdoc Ken Elen and joint postdoc with Antwerp University)/Hasselt University, Prof. Goetheer/Delft University), Zuyd University of Applied Sciences (subcontracting Tim den Hartog, multiple bachelor students as interns) and industrial players in the Netherlands (e.g. via VoltaChem and Brightlands Chemelot Campus) on energy storage in molecular bonds. Following expertise and competence have been developed, and will be deepened and expanded to address the challenges in this ERP:

- Nanoparticle catalyst development and characterization, chemical conversion studies, reaction kinetics and energy conversion efficiency;
- Optical simulation and characterization of nanoparticle catalysts;
- Process and reactor concepts;
- Design and generation of photonic and electrochemical reactor concepts;
- Business case development/economic validation.

The ERP Energy Storage and Conversion activities have resulted and will result in transfer of IP, knowhow and networks to related TNO VPs. The close collaboration in Voltachem, the Interreg projects LUMEN and E2C, the activities at the Brightlands Chemelot Campus and ECCM are good examples for this. Next to that, the living lab developments in Rotterdam and Geleen are accelerated because of the results generated in this ERP.

4. Applications and partnerships

Research line "Photons-to-chemicals"

In the current project, important and unique technology for further exploration in the field of chemical energy storage is acquired, specifically the conversion from CO_2 to CO, CH_4 and CH_3OH. Research on solar water splitting for green H_2 production was started in the framework of this project and continued in 2020 as a separate and dedicated seed-ERP. Such knowledge is valuable for projects aiming at applications in which sunlight needs to be collected and converted into chemical products and fuels. A range of companies located in the Netherlands are interested in solutions for energy storage in molecular bonds, mainly: chemical/fuel producers (e.g. DSM, Shell, SABIC, BASF, Avantium), material/catalyst developers (e.g. Albemarle, Cabot, Kriya Materials, Johnson Matthey, Akzo Nobel, Dow, Nedmag, Sabic, Sibelco). Within the Interreg project LUMEN a user group is formed consisting of several companies who expressed interest in the technology developments (Umicore, Bionerga, Brightlands Chemelot Campus, Borealis, EnergyVille, Tessenderlo Chemie, Aperam, Chemtrix, Signify, Sibelco, CreaFlow). In the framework of the H2020 proposal SPOTLIGHT, the development and validation of photonic devices and chemical process concepts for the sunlight-powered conversion of CO_2 to the chemical fuel CH_4, and the chemical CO as starting materials for production of methanol and higher alkanes will be started. Connection has been made with partners having the necessary competences in photonic devices (Deutsches Zentrum für Luft- und Raumfahrt, EPFL Lausanne, ETH Zürich, Chemtrix, Signify), plasmonic catalysts, chemical processes and assessment of techno-economics and environmental impact to realize an integrated photonic device tailored for sunlight-powered chemical processes and allowing continuous 24/7 operation. Realistic industrial sources for CO_2 and green H_2 will be taken into account via connection with ACEA and Fundación para el Desarrollo de las neuvas technologias del hidrogeno en aragon (FHA). Furthermore, TNO has a strong background in physics and chemistry of colloidal systems, functional coatings and nano-structuring processes like optical and nano-imprint lithography. These competences are used for the design, synthesis and production of nanostructured precision materials and coatings with an optical functionality. ln a variety of applications, TNO has applied tailored nanomaterials for efficient harvesting of sunlight. Thus, the knowledge acquired in the current project is anticipated to be highly significant in this context. It is anticipated that this approach will lead to breakthrough innovations and will significantly contribute to the strengthening of the position of TNO, especially in the Chemical and Energy domains, and in the emerging European Solar Fuels community.

Research line "Electrons-to-chemicals"

TNO will have the unique infrastructure and capability of assessing the technical feasibility of an electrochemically induced transformations, the knowhow on the design of the total system and the possibility to assess economic feasibility. TNO's knowledge position will also lead to a strong European position related to system and process development and to electrochemical transformation of carbon based molecules.

The quality and efficiency of our service will be broadened and improved. Our domain knowledge will be used to establish B2B and sponsoring projects and also to attract programmatic company participation. H2020 projects will be used to further enhance our knowledge position.

Prospects for applications:

1. Shared Innovation Program VoltaChem will be the main marketing & business development channel to interact with market stakeholders, establish an overall open innovation program on electrosynthesis and initiate bilateral spin-off projects.
2. B2B projects. In 2018, already B2B projects have been developed on customer specific specialty applications related to the synthesis of formic acid and in 2019 and 2020 more projects and collaborations were defined which lead to an increased market visibility and unique know-how and infrastructure position in North Western Europe.

3. Subsidized projects, such as RVO and H2020 projects are used to further enhance our knowledge position (e.g. SPIRE10 and projects under TKI Chemie and TKI E&I), especially in the field of paired electrosynthesis and electrochemical CO_2 reduction.
4. Setting up of a Shared Research Program aimed at the integration of CO_2 capture and electrochemical conversion.

It is of importance to note that more than 40 companies are connected via VOLTACHEM or via the Interreg E2C interest group. This leads to an excellent dissemination channel and to strong partner relationships.

An interesting development is the investigation of novel chemical routes which can use CO as reactant and lead to the creation of new end products and the creation of new value chains. Advancing the integrated CO_2 capture and electrochemical conversion of CO_2 also leads to the synthesis of new molecules in addition to formic acid, such as glycolic acid or oxalic acid.

A special academic/industrial committee ECCM (Earl Goetheer is a member of this committee) on instigation of the topsectors HTSM, Energy and Chemistry has been established with the main task to advise the topsectors and the Ministry of Economic Affairs on a multiyear research program on electrochemical solar fuels. TNO is active member of this ECCM committee. ECCM is established as a Key Technology for the KIA/KIC 2018-2019, with strong links to various top sectors, NWA routes, societal challenges and other Key Technologies. There is currently already a strong network between the TNO groups active on solar fuels and the following universities: Utrecht University, Leiden University, Twente University, Eindhoven University of Technology/DIFFER, RWTH Aachen University, Hasselt University, Zuyd University AS and Delft University of Technology, which was established in the framework of the ERP program (exemplified by joint NWO, Interreg (VITO) and TKI projects). Furthermore, experts from the User and Advisory Committees of the Interreg projects and the Chemelot Campus are consulted on a regular basis with respect to technoeconomic feasibility of these processes.

Plan Year 2021

A. Plan – Research Line “Photons-to-Chemicals”

A.1 Key results so far

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 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.

A.2 Key objectives and expected results

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.

Expected essential results 2021

- Lab scale minifactory operational for CH_4 production.
- First stage economic feasibility study for CH_4 production completed and published.
- Plasmonic catalyst for CO production optimized, and results patented and/or published.
- First catalysts designed, developed and validated for photochemical or photoelectrochemical CH_3OH and $C \geq 2$ chemicals/fuels production; implications for reactor mapped.

Intended new partnerships and follow-ups

- H2020 project SOLANOL: develop and consolidate an integrated photoelectrochemical system that can perform methanol synthesis driven by sunlight, through CO_2 reduction associated to CH_4 controlled oxidation, aiming to a "closed carbon cycle".
- H2020 project SPOTLIGHT: develop and validate a photonic device and chemical process concept for the sunlight-powered conversion of CO_2 to chemicals/fuels CO and CH4. Towards demonstration using natural sunlight (TRL 6).
- TKI projects FLUXCHEM (with Chemtrix and Signify) on development of integrated system photoreactor and light source for liquid phase fine chemicals production, and MAT4CAT (with Sibelco) on validation of inorganic materials from Sibelco's product portfolio for CH_4 production.
- Active participation in The International Solar Fuel Forum and Sunergy (continuation from 2020)
- Partnership with academic research group on C≥2 chemicals/fuels production

Intended Dissemination of project results:

- >1 original research article
- 1 minireview/perspective article
- 1 LUMEN newsletter, 1 LUMEN press release
- >2 symposium contributions
- 1 network event LUMEN

B. Plan – Research Line "Electrons-to-Chemicals"

B.1 Key results so far

In the framework of the project, 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 demonstrated that our (patented) approach can also be used for integrated CO_2 capture from air and direct conversion to value added products.
In 2020, we have developed a process and system for integration CO_2 capture from flue gas and air with electrochemical conversion of CO_2 to CO and formic acid, bringing it from TRL2 to TRL 3-4. The Faradaic efficiency for CO and formic acid was above 60%. The carbon efficiency was above 30%. The carbon efficiency can easily be increased by operating the electrolyser at elevated pressures. This will lead as well to higher current densities. An **article** has been drafted to be send to a high ranking journal in August. Moreover, it has been demonstrated that it is possible to convert CO to formaldehyde in a non-aqueous solvent with high efficiencies. This has been **patented** by TNO. Although the main focus was on converting CO_2 to C_1 molecules, it has as well been shown that it is possible to convert CO_2 to a C_4 molecule, tartaric acid. This is the first time that it has been demonstrated that starting from a simple C1 molecule, a highly functionalized molecule is produced. The results of this proof of principle study has been **published** in a peer reviewed journal.

Dedicated separation technology was taken into account by reactor development for the design of a three compartment electrochemical reactor for the continuous removal of formic acid/oxalic acid during conversion of CO_2 towards these products. Within the framework of the Interreg E2C project, a basis of design for pilot unit conversion of pure CO_2 to formic acid was developed. Further focus was on electrochemical reactor design (starting from pure CO_2) . A pilot scale pressurized bench scale unit (Electra) for CO_2 to formic acid was fabricated the design of ~1 kg/hr CO_2 to FA demonstrator has been made, construction will be established in 2021. An optimized reactor design related to mass transfer based on flow promotors and 3D electrodes has been made. This has led to a peer reviewed **article** on process intensification. Moreover, based on the knowledge related to membrane contactor (a topic which TNO was one of the world leaders), a novel gas diffusion electrode architecture has been designed. This new design would enable the scale-up towards industrial relevant scales and conditions. The current designs can be used at lab-scale but scale-up would be difficult. TNOs new approach could solve this problem. This approach has been **patented** this year.

B.2 Key objectives and expected results

In 2021, the ERP will continue to focus on the integration of CO_2 capture with utilization towards fuels and chemicals. The intended system should have to potential to convert CO_2 with an overall faradaic and carbon efficiency above 80%. The key objectives for 2021 are:

1. To develop suitable stable electrode materials for the conversion of the absorbed CO_2 towards C2 molecules (ethylene oxide and ethylene)

2. To develop novel electrode/reactor designs based on gas diffusion electrode (GDE; basis of this has been patented this year) which can be upscaled (ie potential for operating at elevated pressures, should work with non-pure gasses,
3. To develop non-membrane based electrochemical reactor system for the conversion of CO_2 to C1 molecules
4. TRL 4 demonstration integrated capture and conversion

Objective 1: the knowledge obtained related to C1 production in 2020 is expanded towards C2 molecules, which have a considerable higher value. The aim is to achieve proof of principle. Detailed technical-economic evaluation will be done, to determine economic potential. If successful, the envisaged process can be patented by TNO.

Objective 2: A novel GDE architecture has been developed in the ERP of 2020. The aim is to achieve proof of principle. Based on the obtained results scale-up study will be done to implement these kind of materials in advanced electrolysers.

Objective 3: It has been identified that it would be possible (in theory) that you can do an integrated CO2 capture and conversion concept without an ion-exchange membrane. This can lead to a further cost reduction and to robust processes. A solvent/electrolyte system will be optimized to be able to work via this concept. Main challenges are to prevent oxidation of the solvent and products. If successful, the envisaged process can be patented by TNO.

Expected essential results 2021

- 1 kg/hr test installation (ZEUS) commissioned and in operation. Will be used for proof of concept integration CO_2 capture from simulated flue gas with conversion
- Proof of principle of integrating CO capture with electrochemical conversion towards C2 molecules (minimal Faradaic efficiency > 20%)
- Proof of principle non-membrane based reactor system with a potential to be scaled-up afterwards.
- Joint PhD students with TUDELFT on this topic to improve fundamental basis of the by TNOs demonstrated concepts

Intended new partnerships and follow-ups

- TKI toeslag project with DSM ZECEF: TRL4 development CO_2 capture from fermentation integrated with conversion (awarded, 2020)
- H2020 project DIRECTLY (NZE-5): demonstration CO_2 capture from flue gasses and conversion upto TRL 6 by 2023
- MOOI project (TKI): TRL4/5 demonstration CO_2 conversion to CO/formic acid
- H2020 project ECOFERM: TRL 5 demonstration CO_2 capture from fermentation integrated with conversion
- FIELD Lab Rotterdam: electrochemical test street available for industrial collaboration

Intended Dissemination of project results:

- >2 original research article
- >2 patent applications
- >2 conference participations
- Organisation via interreg E2C of a symposium related to CO_2 utilisation

3D Nanomanufacturing Instruments

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

Program description

1. Problem definition

To accommodate the demands for ever smaller, faster and more efficient devices, the semiconductor industry is shifting away from planar device configurations towards 3D or stacked structures and new materials and -properties, still at ever shrinking pitches. These trends are:

- The structures are becoming more complex, from the existing two-dimensional configurations to FinFET (Fin Field-Effect transistor) to LGAA (Lateral Gate-All-Around) and VGAA (Vertical Gate-All-Around).
- The development of shrinkage(half) pitch from now 22nm (metal / 18nm gate to 18nm / 12nm in 2027. At the same time the gate length of the devices is shrinking to 7nm.
- A heterostructure for a vertical FET including new materials which properties need to be measured and characterized.

Hence, smaller, more complex structures and new materials! No doubt the semiconductor industry is facing major challenges on manufacturing, metrology and testing.

To enable the production of these new devices with sufficient yield the development of (non-destructive) techniques that are able to image, measure and characterize nanoscale production features and materials (properties) is needed.

2. Positioning

New metrology tools are required to facilitate the semicon industry to achieve faster, smaller and more (cost) efficient semicon devices. There are various approaches that can be considered. TNO is focusing on Scanning Probe Microscopy (SPM) as one of the promising solutions for measuring defects and dimensions as well as properties of 2D and 3D structures. The reason for focusing on SPM is the non-destructive character, access to directly measured surface (and sub-surface) profiles, the versatility by expanding the technology to different modalities (surface, sub-surface, chemical and quantum), and the operation near the production line. For example, SPM is the believed to be the best suited method to quantify profile, Line-Edge-Roughness, Sidewall Roughness (see table), which are all important parameters in the EPE (Edge Placement Error) budget, which is the leading budget to enable shrink. Furthermore, SPM imaging is possible through optically opaque layers, which is essential because the devices are moving from 2D to 3D structures. Finally, SPM can be extended towards material characterization/ chemical composition at the nano-scale (chemical imaging) and (a.o.) conductivity measurements through quantum sensing.

TNO is frontrunner in SPM-based metrology solutions for the semiconductor industry, in particular for topology and subsurface measurements. Other relevant players are IMEC and companies like ASML (Yieldstar, Holistic Lithography and HMI e-beam), NFI (High Throughput AFM), Bruker and Park (various AFM applications), AMAT and KLA/Tencor (multiple technology solutions, mainly e-beam and optical metrology). Fraunhofer Institute for computational lithography as well as PTB and NIST on scatterometry, Thermofisher for electron microscopy – just to name the more important players in instrumentation and metrology research.

3. Objectives and approach

Subsurface nano-tomography for 400 nm features at a depths up to at least 5 μm. This measurement mode can for example be used to image alignment markers for improved overlay. In the future, the lateral resolution can be decreased by going to higher opto-acoustic frequencies enabling on product metrology. It is believed that with roughly 2 years a party like Nearfield Instruments and/ or ASML can start implementing this technology into a commercial tool. On product metrology will follow later.

Material/ chemical composition. This measurement mode can be used to detect and identify potential contamination and to verify the chemical composition of features with varying material layers. The goal is to reach a resolution of 5 nm and a sensitivity (information limit) of 2 nm, thereby making this technique suitable for semicon applications. It is believed that chemical imaging for contamination control can be made available within roughly 2 years, however application to stress measurements and doping profiles is likely in about 4 years available.

Quantum sensing. This measurement mode can be used to measure (sub)surface features with different conductivity properties, ultimately at a few nm accuracy. These measurements can be used, for example, to detect interconnect defects and to measure the thickness of metallic mask layers and the height of buried features under these layers (e.g., FinFETs). Another application may be to measure the subsurface dopant extension and concentrations and to characterize quantum bits for quantum computing. Mature solutions for all of these applications, however, lies significantly further away in the future, > 5 years.

AI and smart data analyses: it will be researched how AI and smart data analyses could be used for multi-modal imaging and characterization. A first attempt will be made to tailor the hardware system in such a way that the system will optimally serve the AI data interpretation. This approach has been coined design for AI and could enable a new way of working for the system engineering community.

4. Applications and partnerships

Subsurface nano-tomography:

The main application for subsurface nano-tomography is overlay measurement to meet the demands for the upcoming nodes (5nm – 1.5nm). The main partners in this area are ASML and NFI as guiding companies and B2B partners. An impulse program has been stared together with the TU/e including 2 PhD students and a PDEng.

Material/ chemical composition metrology

The driving applications are Leading Edge Roughness (LER key performance indicator) measurement in Directed Self Assembly (DSA) processes, nano-contamination of organic particles (~5 nm) and in the longer term doping profiles of semiconductor materials. Guiding partner for this applications are INTEL (DSA process) and Molecular Vista (hardware configuration). On the academic side the Electro-Magnetic (EM) modelling capabilities of TU/e are connected to this program including 1 PhD student. Also the Plasma and Materials Processing group in the Applied Physics department at TU/e is linked to this part of the program. Next, an anticipated strong link with the Holst Centre is anticipated for Atomic Layer Decomposition (ALD). Finally, chemical composition metrology is TNO's contribution to the EU-project IT2.

Quantum sensing

The leading application for quantum sensing in nano-magnetometry, such as magneto-resistive random-access memory (MRAM) applications (~10nm features). At a later stage, defect inspection through conductivity measurements will follow. Ultimately the investigation on quantum sensing will be part of solid-state q-bit metrology. There is a cooperation with TU Delft, Leiden University, and Qtech in a granted NWA project. As industrial partners, Qnami and Qzabre are connected to the program.

AI and smart data analyses:

Next to smart data analysis, hardware systems can be designed knowing that their data processing is done by AI algorithms The hypothesis is, that these system will perform better than conventionally (manually) designed systems. Design for AI is the Key Enabling Methodology which is developed in this program. Potential partners are Demcon and Applied AI.

Plan Year 2021

A. Plan – Research Line "Subsurface nano-tomography"

A.1 Key results so far

The world's first top actuated GHz scattering based SSPM setup built: >5 GHz piezos designed and successfully fabricated, piezos successfully integrated on custom AFM cantilever, initial sample measurements performed which are not possible with current optical semicon metrology.

A.2 Key objectives and expected results

<u>Optimized SSPM hardware:</u> optimal signal-to-noise ratio, cantilever tip roughness and tip smoothness to increase performance and reproducibility by 25% enabling accurate measurement of the scattered ultrasound field and thus accurate alignment and overlay measurements.

<u>Interpretation/imaging algorithms</u> for complex semicon samples. Higher acoustic frequencies will give more useful spatial information for alignment and overlay determination.

<u>Measurement of a few complex semicon samples</u> – including a 3D NAND sample (providing availability)

An initial experimental exploration of the benefits of <u>multimodal imaging</u> will be performed for relevant semicon samples. Goal is to combine measurement results from different modes to further enhance the accuracy. At least one publication in a peer reviewed journal is expected.

B. Plan – Research Line "Material/ chemical composition metrology"

B.1 Key results so far

All major physical processes leading to contrast in IR-AFM have been modelled – electromagnetic field enhancement, sample heating and expansion and the resulting cantilever dynamics. Together, these results provide insight into the measurements and will guide us how to improve resolution and sensitivity on complex structures. The modelling will be validated experimentally in the remainder of 2020 once the new IR-AFM is installed (Sept 2020). Improving resolution and sensitivity will be continued in the ECSEL EU project IT2.

B.2 Key objectives and expected results

Develop chemical imaging into a suitable and valuable metrology tool for complex, 3D structures with a resolution of < 2nm (the future 2 nm node). We envision that IR-AFM will be used in several ways: for process development of to tune the right process window, and next to (for example) traditional high-throughput optical techniques to periodically assess the process window. Parameters to assess are i.e. micro contamination (< 10nm particles in trenches) and deposition of thin layers on 3D structures.

The insights of ERP 2020 need to be extended to cover complex, 3D structures to enable characterization of all relevant semiconductor structures. This requires fundamental understanding of near field enhancement, optical forces and sample heating in such small spaces. Also requires understanding cantilever dynamics to choose the optimal method to measure these effects.

Key result: <u>demonstrate 10nm resolution on a sidewall</u> (>75 degrees angle) and / or in a confined space (i.e. tip size is significant compared to top opening width).

C. Plan – Research Line "Quantum Sensing"

C.1 Key results so far

<u>Instrument Design:</u> We completed the design of TNO's first proof-of-principle system, able to use a single NV center on a scanning probe to perform high resolution (~10 nm) and ultra-sensitive magnetometry (~1 nT/$\sqrt{Hz}$). The designed system meets the performance of commercial systems while giving us the flexibility to modify it and integrate it with other TNO AFM-based instruments

<u>Instrument Assembly:</u> We estimate to finish the assembly of the state-of-the-art prototype by November 2020, as well as to perform the first characterization.

Two grant applications submitted to the European calls:

- AtomMRI was submitted to the call Emerging paradigms & communities (FETPROACT-EIC-07-2020), in a consortium including pioneers in scanning probe microscopy with NV centers and quantum sensing (University of Ulm, ETH, TU Delft, QuTech, Fraunhofer IOF). The role of TNO in this proposal is to design benchmarking protocols for a novel instrument.
- METRONOME will be submitted ECSEL Joint Undertaking Electronic Components and Systems for European Leadership. In the topic of SPM with NV centers, TNO will work together with Qnami (SME) and Imec on identifying and work on the steps necessary to ease the industrialization of the technique and its use on Semicon metrology.

In addition we submit 1~2 patents regarding the NV SPM.

C.2 Key objectives and expected results

The key objective in 2021 is to evaluate the performance of the proof-of-principle instrument, to test it on MRAM devices (e.g., High density STT-MRAM or MTJ Pillars) and to evaluate the feasibility of other applications. We expect the following results from those activities:

- Demonstration of basic functionalities such as the mapping DC magnetic fields with nT sensitivity, that could be used for mapping contrast in magnetic samples
- Benchmarking our quantum SPM to academic and commercial systems
- Optimization of the resolution, sensitivity, and speed
- Feasibility test for the conductivity measurements required for semiconductor metrology applications (e.g. measuring the metal layer thickness and Fin height in FinFET devices), defect inspection (e.g. metal filled vias and interconnects), and dopant measurements
- Comparison of measurements done with the instrument to other AFM-based modalities (e.g. subsurface)
- Submission of at least 1 patent

Next to the technical work, we will continue positioning TNO in the European Quantum sensing ecosystem, via EU consortia, academic cooperation, and possible B2B leads.

D. Plan – Research Line "AI and smart data analyses"

D.1 Key results so far

A virtual setup of the optical systems is implemented as layers of a complex convolutional neural network. The phase plate (the diffractive optical element, DOE) is an optimizable layer in the network. A wavefront with increased complexity aberrations is propagated in the optical path and the neural network is trained to recover the input aberrations with and without the possibility to act on the phase plate. Efforts are currently spent in improving the performances also for high complexity cases.

D.2 Key objectives and expected results

1) Demonstrator: procurement of Optics elements based on dimensioning of the virtual setup, assembly and test of setup. Experiments with aberrated wave-front via deformable mirror, and the programmable diffractive optical element learning on digital twin of demonstrator and further on demonstrator, and final wave-front parameter retrieval, with and without optimized DOE.

2) Investigate a different use case with interest on the market:

A) AFM Potential use case: determine an optimal sampling for multimodal imaging. With multimodal imaging at each spatial pixel it is necessary to acquire a spectrum of the chosen imaging modality, which is very time consuming. A.I., knowing the analysis procedure and the cost of the various measurement actions, can determine the optimal sampling scheme for providing sufficient information for minimal measurement time.

B) Engineering Potential use-case: tune the frequency response of a phononic crystal, where the local stiffness of a meta material can be adapted in such a way that transmission of frequency bands is rejected or allowed.

Digital Twin for Structural Integrity

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

Program description

1. Problem definition

Our society is depending on the availability of complex macro-structures. Important critical infrastructure is indispensable, e.g. for the supply of energy, transportation, communication, defense and protection against water flooding. Such infrastructures require both stationary macro-structures (e.g. bridge, offshore wind structure, pipeline) and mobile macro-structures (e.g. vehicles, trains). Due to aging of this large amount of structures, there is a growing need for a new generation of more efficient and effective methods and techniques for safeguarding the structural integrity of these existing assets and (re)design of structures.

Our present ability to forecast a structure's integrity and optimize its (re)design, is limited because utilizing in a meaningful way advanced sensor systems, multiscale models and large amounts of relevant heterogeneous data is too complex. With the current way of working, costs are sharply increasing, interruptions for unforeseen maintenance are difficult to prevent and proper levels of safety are under threat. By developing Digital Twins that flexibly integrate physics-based and data-based models with sensoring, data management and artificial intelligence for creating adaptivity and optimization, we enable systematic and easily repeatable assessments and redesign, a way for keeping our critical infrastructure available at feasible cost and minimal environmental impact.

For structural integrity assessment of existing structures we develop and demonstrate methodologies for creating and utilizing Digital Twins (DT) which combine domain knowledge of structures, with monitoring data, data management and analysis techniques, modelling and artificial intelligence. We do that at three related levels of detail (1) a component, (2) a structure, and (3) a network of structures. For the design of structures we focus (4) on material and geometry optimization of components. The development is guided by the following 4 use cases:

(1) *DT Bolted Flange* twinning a bolted flange connection in an offshore wind monopile for optimization during installation and monitoring the connection during lifetime for detecting the need for maintenance.

(2) *DT Steel Bridge* for twinning a steel bridge in the highway network for assessing its safety and monitoring it when the structure approaches its safety limits.

(3) *DT Road Network* for twinning the highway or an urban road network for providing accurate localized information on vehicle loads on structures, such as bridges, in the network.

(4) *DT Design of structure* for twinning (parts of) a composite light-weight military vehicle to accelerate the design process and optimize the design.

2. Positioning

Interest in developing DTs for different domains has greatly increased in the past years across both academia and industry, accompanied by a growth in the number of related publications. Currently most DT applications are in the field of manufacturing. Table 1 presents key features which, mutatis mutandis, are relevant for DTs for existing structures. The present state of the art for these structures is that *exploratory studies* are being conducted addressing *some of the features*. We aim at a *flexible DT development suite and prototypes of DTs* for the three use cases concerning the integrity of existing structures (1-3) *addressing all features* (some more extensively than others). This positions us at the front of the development of DT technology for the integrity of existing structures. Additional specific USPs of our DT systems will be

- ultrasonic sensing: in-situ bolt (bending and torsional) tension stress measurement, and detection of early stage fatigue and zones of plastic deformation using nonlinear ultrasonic techniques.
- fiber optic sensing: distributed strain sensing for steel bridges to create new line-like sensors arrays to significantly increase the coverage area for early detection of fatigue cracks and load / vibration monitoring.
- modelling: FEM models that utilize sensor data and interact with the AI component, as part of DTs.
- AI: efficient creation of surrogate models for machine learning (ML) and ML parameter estimation making DTs adaptive.
- system integration: generic Digital Twin ICT platform that integrates TNO and external components.

Our DT Design of structure is unique in its capabilities for supporting the development of composite structures under high dynamic load. Additional specific USPs are:

- modelling: linking modelling scales and capturing non-linear and highly dynamic behavior.
- supporting experimentation: high dynamic testing procedures for diagnostics and material characterization; instrumented component testing up to failure.
- algorithmic optimization: adaptive machine learning regression for design optimization, multi-fidelity models.

No academic or commercial tools are available that cover these aspects. Closest are developments at Siemens. Its MultiMechanics creates DTs for design with a fast multiscale modelling approach, which however is suited for virtual product testing and not for design of structures under highly dynamic loads (blast, impulse). Its HEEDS is a suite for automatically optimizing a design under a multitude of constraints that may complement our approach for optimization with respect to regular operation conditions. We are in contact to explore cooperation.

3. Objectives and approach

Overall objective: Supporting structural integrity assessment during design and asset management of macro-structures by integrating physics-based and data-based models with sensoring, data management and artificial intelligence in adaptive Digital Twins

Line A. –Digital Twin Technologies

Objective: Flexible IT eco-system for development of Adaptive Digital Twins on structural integrity.

Approach: Our hybrid AI approach 1.0 for adaptivity of our DTs and tool suite 1.0 for Bayesian parameter estimation and model selection will be further developed resulting in version 2.0. The design of the system, including the data platform, hybrid AI approach 1.0, and tool suite 1.0 will be implemented in software with an (almost) zero-programming approach. The resulting implemented systems will be suitable for application on our steel bridge field site and our lab demo of the bolted ring flange. The IT infrastructure will create a flexible, reproducible, and scalable platform connecting data, models (including computational physics, statistics, and machine learning models), and the users.
PhDs & PostDoc: PhD with University of Groningen on adaptivity of digital twins with scalable computational resources; PhD with University of Amsterdam on exa-computing for surrogate modelling to enable AI optimization of estimates of model parameters; a PostDoc will most likely start with UvA on same topic.

Roadmaps: Buildings and Infrastructure, Maritime and Offshore, ICT PMC Cluster Fast and Open Infrastructures – PMC Adaptive Application Platforms and ICT PMC Cluster Data Sharing – PMC D-LiTe.

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

Objective: Focus on modelling and sensing components to be integrated in the DTs.

Approach: We will further develop our models (including computational physics, statistics, and machine learning models) with physics-based and data-driven simulation models so that they can be flexibly applied to different structures and can be connected to the other elements of our DT Steel bridge and DT Bolted connection. In parallel a tool is being developed for (probabilistic) parameter estimation to enable system, load and damage identification. It will be used for steel bridges in 2021 (version 2.0). Specifically for DT Bolted connection we will elaborate the way pre-stress loss and fatigue damage in bolts of a ring flange are incorporated as factors affecting safety. The next step for our ultrasonic sensing technology will be a proof of principle, followed by incorporation in lab demo DT Bolted connection. Our fibre optic technology for distributed, multi-parameter sensing will be validated in practice at the field site DT Steel bridge.

PhD #Johan HiMat voorstel.

Roadmaps Buildings and Infrastructure, Maritime and Offshore, Wind Energy

Line C. Existing structures: network - Vehicle load

Objective: Digital Twin Road network that updates its information on traffic loads from distributed data sources and can be used to explore future vehicle loads. It enables more accurate assessment of the structural integrity of structures in the network and their expected lifetime. Demonstrated on highway or an urban road network.

Approach: The components for estimating the loads at each point in the network will be integrated in a system with a GUI and facilities for exploring scenario's. The load estimation will be further improved by connecting the system to traffic models. Furthermore, the accuracy of our bridge weight-in-motion system will be further improved, and, as an intermediate step towards its integration in the DT Road network, it will be incorporated in the field site for our DT Steel bridge.

Roadmaps Buildings and Infrastructure.

Line D. Design of structures

Objectives: Digital Twin Design of structures that accelerates and optimizes the design of composite structures. Demonstration of the DT for parts of a composite military vehicle (underbelly, doors).

Approach: Based on experimentally validated numerical models at different scales a DT for design of composite structures is developed. A first version is demonstrated for the optimization of a design of a blast protector panel. Since the numerical models are very computationally expensive due to a highly non-linear behavior, a machine learning supported optimization algorithm is adopted. After proof of principle of the machine learning-supported process, the DT will be extended to the higher modelling scale. It will challenge the first version of the DT by increasing the design space and adding computational complexity. Due to the increasing computational demand we plan to explore high performance computing in order to reduce wall clock time to a reasonable value. The result will be a second version of the machine learning supported DT which is more generically applicable.

PhD: Two NWO proposals for PhD positions at TU Delft have been prepared on multiscale modelling of composite interface and on machine learning supported test procedures.

Roadmaps Protection, Munitions and Weapons

4. Applications and partnerships

Applications have been discussed in section 1 ‘Problem definition’ and per research line in the objectives of the research lines in section 3 ‘Objectives and approach’. We cooperate with partners:

*Line A & B. Existing structures: structure/component – A. DT Technologies & B. Modelling & Sensing.*_**Uni’s**: University of Amsterdam, SURF, TU Eindhoven, TU Delft, Universiteit Groningen, Universiteit Hannover (Leibniz); **RTOs**: Bundesanstalt für Materialforschung und -prüfung (BAM), Deltares, NTNU, Fraunhofer; **Industy**: Akselos, Grow, Amonics; Ferrovial Agroman, Mostostal, IBM, MS Azure; **Governmental**: RWS,

Line C. Existing structures: network vehicle load **Uni’s**: ; **RTOs**: Iffstar; **Governmental**: RWS, Amsterdam *Line D. Design of structures*_**Uni’s**: TU Delft; **RTOs**: Netherlands Aerospace Centre (NLR); **Industy** Solico, Kraus-Maffei Wegmann (KMW), Nexter, IVECO; **Governmental**: Min of Defense, Eur. Defense Alliance

Plan Year 2021

A. Plan – Research Line A. Existing structures: structure/component - DT Technologies

A.1 Key results so far

- requirements document use case ‘Steel Bridge’, reference IT Architecture and System design 1.0
- components from Cloud Native Computing Foundation (CNCF) that fit the designed architecture
- data platform design; basics in place for raw data management and processing
- hybrid AI approach 1.0 for adaptivity of the general DT framework for individual structures
- tool suite 1.0 for Bayesian parameter and boundary condition estimates updating
- computation speed-up through hardware (IT, parallelization) and software (smart algorithms, AI).

A.2 Key objectives and expected results

- Prototype implementation DT Steel bridge, with data platform, hybrid AI approach 1.0 and tool suite 1.0
- additional system flexibility by adaptivity of model interfacing, automated tuning of parameters and selecting models for particular cases and scalability of computing power
- AI approach 2.0 moving from hybrid (physics-based models with tuning of parameters) to data-centered
- tool suite 2.0 for Bayesian parameter and boundary condition estimates updating
- system design DT Bolted connection based on the design of DT Steel bridge
- toolkit enabled by exascale computing to compose virtual bridges for exploring optimal sensor type and placement, and the type of anomaly signal in case of deterioration

B. Plan – Research Line B. Existing structures: structure/component – Modelling & Sensing

B.1 Key results so far

- existing and AI based model components combined for system identification of a bolted connection.
- ultrasonic sensing for pre-stress assessment and fatigue damage monitoring of bolts
- Python toolbox version 1.0 for parameter estimation of (steel) bridges
- system & load identification combining measurement data and FEA for test case Bridge 705

- system identification combining measurement data and FEA for test case IJsselbrug
- distributed fiber optic sensing for dynamic strain sensing (vibration & load) with shorter gauge lengths to increase the number of sensors in the (fiber optic) sensor line
- table top demo of a digital twin for a bridge (with Bundesanstalt für Materialforschung und -prüfung) showing real time system identification and damage detection.

B.2 Key objectives and expected results

- 3D ring flange model calibrated with improved stress measurement and validated by lab test
- Python toolbox version 2.0 for parameter estimation as a unified platform for system, load, and damage identification of the use cases steel bridge and bolted joints.
- proof in practice of fiber optic system for static and dynamics distributed strain measurements with easy to install cable for the use case steel bridge
- proof of principle of ultrasonic sensing system for pre-stress assessment of bolts in ring flange.
- method for quantifying uncertainties and Bayesian updating on the basis of sensor data
- elaborated table top demo with BAM on the Hannover Messe in 2021, start field site DT Steel bridge and lab demo DT Bolted connection.

C. Plan – Research Line C. Existing structures: network vehicle load

C.1 Key results so far

Load map: interactive GIS-tool for traffic load information

- prototype available
- value-of-information of additional data-sources
- interpolation methods and uncertainty quantification

Bridge-WIM: bridge for truck weights

- proof-of-principle available
- points of improvement identified and prioritized
- application scenario's (stand-alone, add-on) investigated

C.2 Key objectives and expected results

Load map: combining sources to reduce uncertainty

- adding data source(s) improving accuracy of the load map
- further develop predictive model in loadmap improving accuracy

Bridge-WIM: bridge as a versatile scale for trucks

- improvement of accuracy so that it meets requirements
- generalize tool for application on any monitored bridge
- integrate with load map and Digital Twin of specific structure

D. Plan – Research Line D. Design of structures

D.1 Key results so far

- validated machine learning supported design methodology for laminate composition
- instrumented blast panel testing device and interface testing procedure for impact conditions
- calibration data on pressure and strain rate dependency
- composite material solution (patent pending) further optimized

D.2 Key objectives and expected results

- incorporation of macro level modelling into machine learning supported optimization
- extension of the machine learning supported design tool for macroscale design with structural aspects
- further validation of composite behavior to improve reliability of physical models and in turn to reduce the uncertainty in the simulation driven optimization

Personalised Health

ERP Contacts: M. van Erk (Project Lead), S. Wopereis & A. Boorsma (Lead Scientists), P. Bongers (Science Director)

Program description

1. Problem definition

A huge increase in chronic lifestyle related diseases puts and enormous burden on the current healthcare system that is not equipped to take care of this problem. Fortunately, lifestyle related diseases are to a large part preventable, manageable and curable; evidence is mounting that lifestyle changes have a profound effect on disease progression and even disease cure is possible. However, changing lifestyle is difficult; therefore, personalisation, i.e. tailoring to an individual's needs and preferences, is an crucial factor for achieving sustainable healthy lifestyle habits. To alleviate the burden of chronic lifestyle-related diseases, a focus on health instead of disease and a more personalised approach instead of an one-size-fits-all approach are essential.

The **biology research line** in ERP Personalised Health focuses on low-grade chronic inflammation, a fundamental process in the development and progress of chronic lifestyle related diseases that manifests into co-morbidities and complications. The research line aims to build the biological knowledge basis for prevention, reversal and cure for diseases with a chronic inflammatory component. To sustain optimization of personal health, new research methodology is needed. The research **methodology research line** focuses on the technical, behavioral and social aspects of personalised lifestyle diagnosis and intervention. 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.

2. Positioning

Optimizing and maintaining health is very relevant within the ageing population and the 24-hour economy. Improving health contributes to a higher quality of life, increased productivity at work, and decreased economic burden. In addition, consumers are becoming more health conscious (Hanspal, 2017), which provides opportunities for innovations in health services and products.

Personalised health, in terms of prevention and health optimization can complement and extend current public health lifestyle recommendations by tailoring lifestyle advice, services and products to the health status, behaviours, preferences and goals of an individual. Scientific evidence shows that a personalised approach is more effective in changing lifestyle behaviours than 'generic' advice, and that they can induce consistent and sustained positive change in health (Zeevi et al., 2015, Cell; Celis-Morales C et al., Int J Epidemiol. 2016; Doets EL et al. Physiol Behav. 2019).

TNO is recognized internationally as expert in the area of personalised health, e.g. through the PhenFlex challenge test as a tool to measure health as flexibility or resilience to a (metabolic) challenge. Additionally, our uniqueness rests in our multidisciplinary approach to health and our systems view on health, including psychological wellbeing, social context, as well as the potential of personal health data and e-health. This ERP will result in a dashboard of tools and technologies aimed at personalized optimization of health. These tools and technologies will be further developed in TNO's roadmaps and (PPS-)projects.

As quoted by Prof. H. Pijl, internist-endocrinologist and Professor of Diabetology at LUMC "TNO has been a leader in Personalized Health already for years. TNO's research in the field of interactions between nutrition and our genetic architecture is amongst the international top. Phenotyping of people with type 2 diabetes - or diabetyping - is innovative and personalizes the treatment of this disease. The great social involvement of the TNO team makes the research quickly applicable and therefore extra valuable."

As quoted by Dr. Josh Anthony, former Vice President, Global R&D, Nutrition and Health at the Campbell Soup Company & CSO of personal nutrition company Habit LLC: "TNO researchers are global leaders in the science of personalized nutrition and their know-how and consumer understanding was necessary to move Habit from concept to launch in just six months. While TNO is unique in their understanding and application of the science of personalized nutrition, they are also unique in their understanding of how to address the challenges of implementation of personalized programs in the marketplace. "

3. Objectives and approach

The objectives of ERP Personalized Health are to develop a) the biological knowledge base for health optimization; b) innovative research methodology to allow for personalization to sustain health and c) to deliver a proof of concept of this multidisciplinary evidence based methodology and knowledge.

In order to meet these objectives, ERP PH has three research lines.

Research line 1: biology innovation

The biology innovation is targeted towards the new concept of elucidation of curbing low-grade chronic inflammation by lifestyle modulation. Therefore the PhenFlex challenge test technology (as developed by TNO) is applied for detection of disturbed inflammatory resilience via quantification of dynamical inflammatory response profiles. In addition, detection of disbalance of mycobiome as a potentially important factor in low-grade chronic inflammation is taken in account. By 2022, we will have developed new personalized intervention strategies to measure and optimize inflammatory resilience and thereby reverse and cure lifestyle related diseases. Within this ERP, the combination of metabolic knowledge with innovative knowledge and application of inflammation will take the personalized systemic approach of health optimization to a next level.

Research line 2: research methodology innovation

The research methodology innovation is targeted towards sustainable health optimization. This research line has 3 focus areas: a) the Personal Health Advice System (PHAS) to standardize and automate personalized health advices; b) valorisation of personal health data; and c) a systems toolbox for sustainable behavioral change. By 2022 we aim to develop 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 including evidence based behavioral change technology. Innovations in the PHAS comprise 1) the innovative way to combine biological, behavioral and socio-psychological diagnostics and interventions in one system and 2) the new hybrid modeling techniques.

In addition we initiate, facilitate, and test “personal health data valorisation”. 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 by setting-up the building blocks for systems-based behavioral change tooling. By 2022, this will have resulted in a systems toolbox for sustainable behavioral change exploiting bio-socio-psycho-environmental aspects. Hannah Regeer’s PhD project (collaboration TNO, LUMC, UMCG) on the effectiveness of a combined community and self-management e-coaching intervention to improved lifestyle self-management among type 2 diabetes patients is part of this research line.

Research line 3: the human proof-of-concept (hPoC) study

Starting in 2020, research lines biology innovation and research methodology innovation will converge in the third research line: the human proof-of-concept (hPoC) study. This research line will integrate the developed biological knowledge and research methodology innovations in a human volunteer study to test the applicability and added value of these innovations in real life. The hPoC will be a combination of a technical and a scientific demonstrator with focus on the multidisciplinary integration.

4. Applications and partnerships

Applications

The PH program delivers services and applications that are of interest for various partners and customers. In the biological innovation research line the following applications were developed:

- A mouse study model for organ inflammation studies.
- Systems Biology Intelligence - workflow for identification of mechanism based biomarkers and intervention targets
- TargetTri – workflow for identification of novel nutritional ingredients specifically targeting adipose and liver tissue
- MyScreen for in-vitro identification of compounds targeting inflammatory robustness through modulating the mycobiome
- Challenge tests for measuring health
- Diagnostic biomarker panel for inflammatory resilience

In the methodology research line the following applications were developed:

- Standardization of the Personal Health Advice system
- Automated health services for lifestyle interventions
- Hybrid Machine Learning models based on lifestyle and behavioral data

- Automated Destillation &Matching models for application of sustainable behavioral change techniques in personalized health.
- Governance models for fair use of personal health data
- Models for building patient communities

In the research line hPoC, the following ERP assets will be demonstrated, integrated and applied:

- Ontology based personalized health advice system, with a 360° view on health, not only focusing on biology, but also on behaviour and personal characteristics;
- Personalized behaviour change support using extended & blended care;
- Personalized lifestyle advice based on phenotypic flexibility and challenge testing;
- Demonstrate improvements in liver and adipose tissue inflammatory status and mycobiome in human as a result of a combined lifestyle intervention;

Internal and External connections

This ERP interacts and collaborates with ERP Applied AI, ERP ExpoSense, ERP Organ-on-a-chip and ERP Body Brain interaction. Output of ERP PH is absorbed in the roadmap Biomedical Health (PMC2, 16, 17 and new PMC Prevention 2.0), Digital Health Technologies (PMC 2-4) and Prevention Work and Health. Parts of the applications developed by ERP Personalized Health are being applied and developed further at B2B projects with Johnson&Johnson, Juvenescence, By-Health and in collaborations (Stevenshof, SLIMMER and the Netherlands Innovation Center for Lifestyle Medicine) and PPS programs (No-Guts-No-Glory, GlucoInsight, Diablend, muscle health, PhenFlex-2, SIDN project, Connect2HealthConsumer, TrustedWorld of Corona, Health Data Community).

ERP Personalized Health connects very well with several routes of the NWA: 025: Creating value through responsible access to and use of big data; 006: Health care research, sickness prevention and treatment; 017: Personalised medicine: the individual at the centre. Tools and technology are incorporated in a number of NWA research proposals (resulting in new PhD-projects). The research focus of ERP PH contributes to the central mission 'Langer gezond' and also to the dedicated missions 'Leefstijl en leefomgeving' 1. Also the research aligns with the activities in the KIA 'Gezondheid en zorg' 2020-2023 of Topsector LSH. The digitalisation co-created in the ERP program and the biological knowledge helps in the further development of the Dutch 'sleutel technologieen' (as defined by the government): digital and life-science technologies. These developments are streamlined with the work in DTL (Dutch Techcentre for the Life sciences), FNH-RI and HealthRI.

1 https://www.health-holland.com/public/publications/missiedocument/missiedocument-gezondheid-en-zorg.pdf

Plan Year 2021

A. Line "Biology Innovation" – Key results so far

Research line biological innovation will obtain knowledge about new personalized intervention strategies to optimize low-grade inflammatory resilience. Low grade chronic inflammation is the key process that is common to all chronic lifestyle related diseases. Being able to treat or reverse low grade inflammation is therefore of great interest to industrial companies as well as to society and health care. The figure below represents the knowledge and innovation areas that WP1 started in 2018, of which most of the work will be finished at the end of 2020.

Key results so far of this research line include:

1. The successful results of the proof of concept mouse study (mPoC) provided first proof for organ inflammation reversal which was strongest for the combined lifestyle intervention (healthy diet + exercise). This forms the basis for the intervention of the hPOC study to be conducted in 2021. In 2020, pathway analyses using Next Generation Sequencing for liver and adipose tissue were performed to unravel the underlying mechanisms. At the end of 2020, the study will be completed with measurements of the innovative biomarker panels in mouse plasma and a draft manuscript of the mPOC study describing all findings.

2. A refined Systems Biology Intelligence (SBI) workflow was developed to select 1) innovative biomarkers reflective of liver and adipose tissue inflammation for the mPoC and hPoC studies and 2) targets for novel mechanism-based nutritional interventions (task 3). At the end of 2020, a draft SBI manuscript will be ready, describing the SBI workflow and verification of the innovative biomarker panel in mouse and human samples.

3. A workstream has been developed for the identification of novel mechanism-based nutritional ingredients to improve inflammatory robustness. Based on the SBI network (task 2), upstream targets for liver and adipose inflammatory mechanisms can be identified, which serve as input for TargetTri to identify novel nutritional ingredients specifically targeting adipose and liver tissue. Some of the identified nutritional compounds will also be tested with the MyScreen platform (task 4).

4. The Mycobiome screening technique (MyScreen) has been set-up, allowing the screening of compounds on Candida albicans growth, which is a fungi that under certain circumstances, such as reduced inflammatory robustness, can cause a fungi infection. At the end of 2020 we expect to have positive results on MyScreen platform with first indications for inhibitory effects of natural (dietary) compounds.

5. An innovative diagnostic biomarker panel for inflammatory resilience using challenge testing has been developed. In collaboration with PPS PhenFlex-2, biobank samples of two caloric restriction studies were used to validate the biomarker panel in detecting effects of caloric restriction on inflammatory resilience of adipose, liver, and vasculature. This developed diagnostics will also be used in the hPoC of 2021 to understand the added effect of exercise on inflammatory resilience.

B. Line "Research and Methodology Innovation" – Key results so far

To achieve personalized health optimization, innovation of research methodology is essential. This research line has 3 focus areas: a) the Personal Health Advice System (PHAS); b) valorisation of personal health data; and c) a systems toolbox for sustainable behavioral change. Key results so far of this research line are described below for each of the focus areas.

A) Personal Health Advice System (PHAS)

PHAS building blocks are defined, which makes it possible to more easily develop Personalized Health advise solutions based on specific (client) questions. Several clients are interested, such as Roche (a PPS project has started in the Roadmap Digital Health), Novartis, J&J and AstraZeneca.

In 2020 access to the cohort data of Lifelines was obtained. Analysis of data from this longitudinal health cohort will focus on Bio-Psycho-Social subtypes in relation to lifestyle changes. The data has been cleaned and prepared for analysis. Additionally, in collaboration with ERP AI we have used these data to develop ways to learn on data that are distributed over different locations (Federated Learning).

B) Valorisation of health data: Due to the covid-19 crisis some activities had to be adapted: a workshop that was scheduled was postponed. A new plan that involved a proposal for the SIDN-fund was written and awarded! This new opportunity enables a hands-on approach to develop governance rules for a health cooperative and dynamic consent modules for a patient group with chronic disease.

C) A systems toolbox for sustainable behavioral change

- A paper is written on technology acceptance of self-management eCoach, a study conducted among 92 Type 2 Diabetes patients and submitted to the Journal of Medical Internet Research.

- Behavioural change techniques have been reviewed and translated in practical strategies, focussing on behavioural maintenance. These include strategies on stress and mood management, intrinsically motivating strategies (identity, values and reinforcement), self-confidence strategies, planning strategies and (instrumental, emotional and practical) social support strategies.

- These techniques have been embedded as part of the N-1 pilot study. In addition, an ontology-based translation has been made for inclusion in the digital PHAS.

- A protocol has been written for the N-of-1 pilot study to promote individualised sustainable behaviour change to promote physical activity, healthy diet and weight reduction. The pilot study is an example of a blended care support strategy, combining monitoring devices with self-management and coaching support. Key to the study is that based on individual monitoring of behavioural progress, individual coaching trajectories are set up. The pilot will be conducted together with a type 2 diabetes patient community (JeLeefstijlAlsMedicijn). The study has been given approval from the research evaluation committee and recruitment of the participants has started. The study will start in the first week of September 2020.

C. Line "hPoC study" – Key results so far

In 2020 we have started research line 3 'hPoC study'. The human proof of concept (hPoC) study is a scientific and technical demonstrator, to test in real life the integration of the various parts, technologies and knowledge that have been developed during the first three years of this ERP. The innovations that will be implemented will relate to personalised diagnosis and feedback on health and a personalised intervention program to optimize health, offered in blended care setting (combination of digital and face-to-face). Key milestones and results in 2020 include the study design, the study protocol and approval of the study by the Medical Ethical Committee (METC). The study set-up has been created and discussed with members of research line 1 and 2, as well as with business developers for an outlook on how the demonstrator can help with valorisation after ERP PH duration. An overview of the proposed hPOC study design is included below. At the end of 2020 we aim to have medical ethical approval, in order to start the recruitment of participants and adhere to the planning of the study execution in 2021.

Key objectives and expected results for ERP Personalised Health in 2021

2021 will be the final year of this ERP. The key objectives are the successful completion and dissemination of the different activities from research lines 1 and 2. In addition, the last year will be a challenging endeavor that focuses on the conduct of the human proof of concept study. This is an essential validation step that brings all different results together demonstrating the applicability and scalability of the developed technology and knowledge.

We have two hypotheses that will be tested in the hPoC, these are:

1) Personalised tools and technologies help to stimulate a healthy lifestyle in people with overweight and/or obesity and who are cardio-metabolically compromised;

2) A personalised combined lifestyle intervention (in Dutch: GLI = gecombineerde leefstijl interventie) can reduce low-grade inflammation in people with overweight and/or obesity who are cardio-metabolically compromised

We focus on a preventative setting and will include men and women (a total of ~n=60 per arm), aged 40-70 years, with overweight and impaired fasting glucose (but no type-2 diabetes) and/or obesity (BMI 30-40) and increased low-grade inflammatory markers. The study group will get a personalised GLI (personalised-SLIMMER) with the following personalised add-ons:

1) a personal feedback based on 360° feedback on biology, personality and behavior;

2) personalized diet (low-caloric diet; low-carbohydrate diet; Mediterranean diet or intermittent fasting) and exercise (cardio; resistance; free choice) advices via ontology based PHAS based on PhenFlex data and other health parameters;

3) intermediate feedback based on lab values and behavior via PHAS (goal achievement; self-monitoring; self-measurements);

4) personalized behavior support via e-health (ontology based reasoning via personalized feedback and behavior change exercise)

5) coaching (extended & blended care to digitally support coach and participant to reach short-term and long-term lifestyle change).

This personalised SLIMMER intervention will be compared to the existing accredited combined lifestyle program ‘SLIMMER’. The personalised add-ons and the increased and specific coaching tools, may ease lifestyle behavior change adherence for subjects compared to the standard GLI. The effectiveness of personalizing SLIMMER and improved coaching strategies, will be examined with the Phenflex challenge for metabolic and inflammatory response before and after the six months intervention period. In 2021, we aim to conduct the study, analyse the blood and stool samples, analyse and interpret the data and write a draft publication.

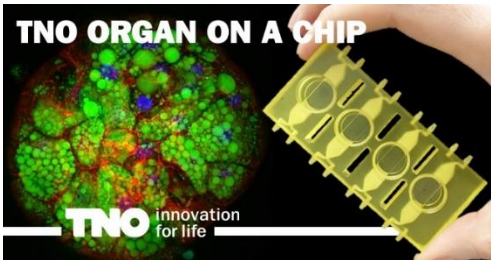
Organ on a Chip

ERP Contacts: I. Bobeldijk (Project Lead), E. van de Steeg, Geurt Stokman (Lead Scientists), P. Bongers (1st Science Director)

Program description

1. Problem definition

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.



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.

2. Positioning

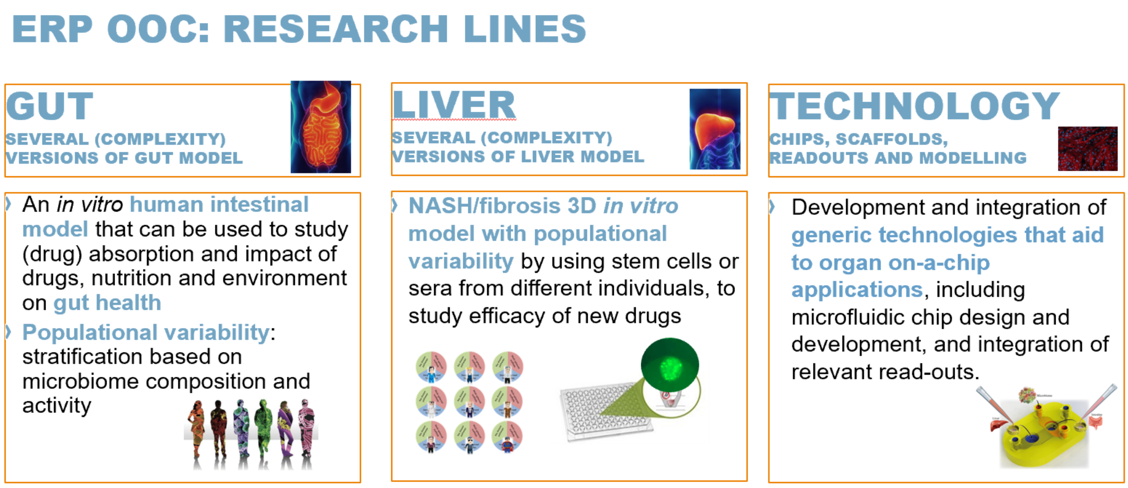
The main goal of this ERP is to contribute to the development of stratified and/or personalized interventions by developing the concept of **population on-a-chip**. By 2023 we will develop a (stem-cell based) in vitro pre-clinical toolbox with integrated readouts, enabling the introduction of population 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. 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.

3. Objectives and approach

The objective of the ERP 'Organ on chip program' is to improve the development of better predictive, more physiological (personalized) human stem-cell based *in vitro* models that will enable 'population on-a-chip' development. We distinguish so called "**organ function on-a-chip models**", which are complex, multicellular (stem cell based) microfluidic models representing functionalities of a specific organ, and the concept "**population on-a-chip**", in which these organ on-a-chip models are expended to study interindividual and populational variation by application of stem cells from various individuals and combination of healthy donor cells with individual sera or microbiota. With these models we will help pharmaceutical industry to lower the attrition rates in drug development, thus lowering the development costs and time to market as well as help both pharmaceutical and food industry to develop stratified and in the end personalised interventions for treatment of different metabolic and immune health dysfunctions.

4. Applications and partnerships

Our program focuses on tissues and disease areas in which TNO has extensive knowledge, experience, and market position ("right to play"), and develops validated applications relevant for pharmaceutical and nutrition industry.



Gut: develop and implement advanced in vitro human intestinal models that can be used to study drug absorption and the impact of drugs, nutrition and environment on gut health.

Liver: focus on addressing patient variability already in preclinical efficacy screening using advanced cell models. The approach will be by using stem cells from more individuals (mimicking the population variability in the clinical trial phase) or by using serum from individuals/patients and primary hepatic cells.

Technology: focus on the development of organ on-a-chip hardware which is easily used in industrial applications (tissue explants, cell based barrier models and organoids), and which will enable the organ on-a-chip and population on-a-chip applications.

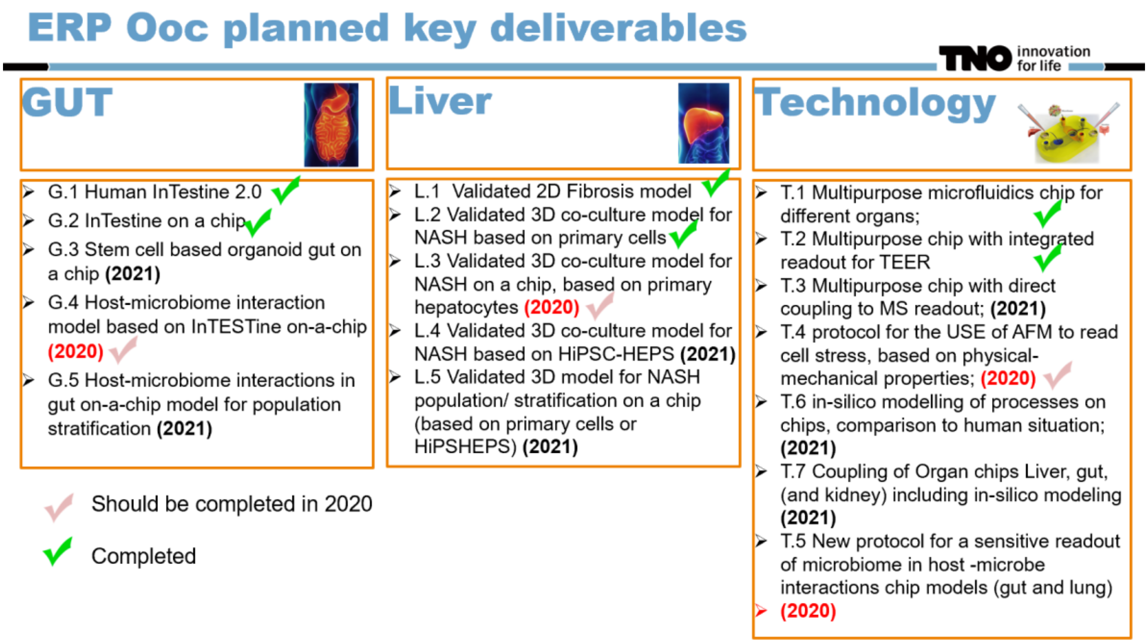
In our development, we collaborate with different internal and external collaborators.

Internal: Within Unit Healthy Living, departments MSB, MHR and Rapid are involved. We collaborate with Units Industry (development of sensors) and CEE (planned applications of the models in different projects). We are part of several consortia, developing organ on a chip technology and applications, hDMT, collaboration with Twente. Specific external collaborations, established, new and planned are shown in the figure here above.

Plan Year 2021

Deliverables for 2021 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.

Overview of the key results achieved until 2020 is shown in the figure below.



A. Plan – Gut function on a chip

A.1 Key results so far: Figure for key results.

A.2 Key objectives and expected results

In 2021 we will focus on achieving populational differences by applying stem-cell derived organoids from multiple donors and combination with (personalized) microbiota. Furthermore, market and implementation plans will be [prepared in order to ensure timely implementation of the developed models in the roadmap BMH, PMC in-vitro models.

Expected essential results 2021:

- G.3 Stem-cell based intestinal organoids implemented in microfluidic chip
  - Protocol culturing cells on a chip with Caco-cells
  - Proof of concept stem-cell based cultures on a chip (with MatTek)
  - Proof of concept 2D gut organoids on a chip
- G.5 Validation of host-microbiome interactions in the Intestinal Explant Barrier Chip (IEBC) model for studying populational differences in relation to pharma and food interventions
  - Validated model for gut host-microbiome interactions using the aerobe-anaerobe interface using gut tissue (patent 2020)
  - Democase aerobic-anaerobic interface box for applications outside of TNO (patent 2020)
  - Demonstration of populational differences in gut function using the gut on a chip model
- Implementation plan for in the roadmap and dissemination
  - Overview of the necessary technology developments after 2021
  - Overview of the necessary validations/ democases
  - Essential collaborators, grant submission plan (where possible), Company contact plan
  - At least one manuscript Intestine on a chip, several presentations on different conferences

Intended new partnerships and follow-ups:

- B2B projects with pharmaceutical and food industry, several negotiations ongoing
- MatTek- collaboration in developing proof of concept stem-cell based gut cell cultures on a chip
- Implementation in roadmap BMH and PMC – further development of specific market applications (e.g infant formula, disease modeling (Chrohn's disease)

B. Plan – Liver Function on a chip

B.1 Key results so far: Figure for key results.

B.2 Key objectives and expected results

In 2021 we will focus on the introduction and validation of the use of human iPSC (stem cell)-derived hepatocytes in the static and microfluidic model set-ups, intended for replacement of primary hepatocytes, these steps will lead to a refined population on a chip with respect to the liver model.

Expected essential results 2021

- L4: Validated 3D co-culture model for NASH based on HiPSC-HEPS
    - Final protocol for model
- L5: validated 3D model for NASH population on a CHIP
    - Functional effects of distinct genetic polymorphisms on therapeutic efficiency of (prototype) drugs within the context of diet-induced fibrosis
    - Demonstration of effects of combination drug therapies based on individual polymorphism profiles on a chip
- Implementation plan for in the roadmap and dissemination
    - Overview of the necessary technology developments after 2021
    - Overview of the necessary validations/ demo-cases
    - Essential collaborators, grant submission plan (where possible), Company contact plan
    - Manuscript describing the static 3D model and its validation with model drugs
    - Several presentations at conferences

Intended new partnerships and follow-ups

- With academic partners, possibly within the NECST at Leiden BioScience Park: iPSC biobanking and creation of isogenic iPSC-derived hepatocytes for focus on distinct polymorphism without genetic background noise
- With mid-size – large pharma: fee-for-service studies possibly in combination with animal studies
- Development of high-throughput analysis tools: advanced Raman spectroscopy, other developments within TNO

C. Plan – Technology Organ on a Chip

C.1 Key results so far: Figure for key results.

C.2 Key objectives and expected results

Development and integration of generic technologies that aid to organ on-a-chip applications, including microfluidic chip design and development, and integration of relevant read-outs.

Expected essential results 2021

- T.3 Multipurpose chip with direct coupling to MS readout;
    - Additional readouts for both the cell and the biopsy chips
    - MS coupling is not feasible in 2021
    - Market analysis for selling the developed chip/ service
- T.6 in-silico modelling of processes on chips, comparison to human situation;
    - Models and experimental designs for gut-Liver coupling
- T.7 Coupling of Organ chips Liver, gut, (and kidney) including in-silico modeling
    - First demonstrator coupling of liver and gut, incl. in-silico models
    - First demonstrator gut- kidney, incl. in silico models
- T.5 New protocol for a sensitive readout of microbiome in host -microbe interactions chip models (gut and lung)
    - RNA isolation and sequencing protocol
    - Democase with LUMC lung-on-a chip model
- Implementation plan for in the roadmap
    - Overview of the necessary technology developments after 2021
    - Overview of the necessary validations/ democases
    - Essential collaborators, grant submission plan (where possible), Company contact plan

Intended new partnerships and follow-ups

- Fujifilm, Kao à application of IBC in house (license)
- TTW SMART grant application, TU Twente & others > 2021

Submicron Composites

ERP Contacts: A. Wypkema, P. Buskens & T. ten Cate (Lead Scientists), C. Hooijer (Science Director)

Program description

1. Problem definition

General: The overall goal of this ERP is to develop materials with tailored functionality, by controlling their micro- and/or nano-structure and chemical composition. We aim to progress from state of the art monofunctional materials via materials with multiple passive functionalities to active and adaptive materials. We demonstrate the knowledge gained in use cases chosen in collaboration with Brightlands Materials Center and its partners in the Sustainable Buildings and Additive Manufacturing programs.

Sustainable Buildings research line within the ERP: The first goal is to develop nanocomposite glass coatings and polymer nanocomposite films for glass lamination, to improve the energy efficiency of buildings. Focus of the ERP until 2023 is on thermochromic nanocomposite coatings and films, that can rapidly switch from solar heat transmission to heat blocking and *vice versa* at a temperature between 15°C and 25°C. Such coatings/films bring additional (to current state of the art low-emissivity coatings) energy savings up to 15% for intermediate climates such as The Netherlands. *Ergo*, this significantly contributes to realizing the sustainable energy and climate targets, specifically for the built environment. The second goal is to develop coatings and films that capture part of the sunlight that falls on a window, and guide it to the frame of the insulating glass unit in which small photovoltaic modules are integrated for light-to-electricity conversion.

Additive Manufacturing research line within the ERP: The overall goal is to develop materials and processing technologies for the 3D printing of (continuous) fiber reinforced polymers into complexly shaped products that can replace metal products, e.g. lightweight brackets, hinges and structural components for aerospace or replacement of obsolete parts in transport applications. Replacing metal components by polymer composites leads up to 50% in weight reduction for the same strength, resulting in reduced energy consumption in transport applications. For example, each kg of weight reduction in aeronautic applications leads to a reduction of 1000 L of kerosene per year. Processing composites in complex shapes with conventional technologies is difficult and expensive due to need for complex moulds and many manual process steps. Therefore, the use of additive manufacturing is preferred, especially for small and medium sized series, and can also be used in integrate multiple functionalities to even further lower the weight and volume of products.

2. Positioning

Sustainable Buildings research line within the ERP: A recent study, commissioned by Glass for Europe and performed by TNO has shown that by equipping all buildings in Europe with energy-efficient glazing, the total energy consumption of buildings can be reduced by over 30% for most countries. Current commercially available double or triple glazing products typically have a reduced thermal transmittance, and avoid loss of radiator heat (= infrared radiation of a wavelength of 2.5 µm – 10 µm) through use of low-emissivity coatings. Thermochromic materials, which are not yet commercially available, are complementary to low emissivity coatings, since they regulate the shorter wavelength infrared radiation from the sun (wavelength 750 nm – 2.5 µm). Thermochromics can switch their solar infrared properties from transmissive to blocking and vice versa depending on the glazing temperature (Fig. 1). Due to this self-adaptive property, which promises huge benefits in intermediate climate regions, thermochromics have been subject of many academic studies in recent decades. Within this ERP research line, we primarily focus on the development and demonstration of thermochromic nanocomposite coatings and films, that can switch from solar heat transmission to solar heat blocking and *vice versa* at a temperature between 15°C and 25°C. Such coatings/films bring additional (to current state of the art low-emissivity coatings) energy savings up to 15% for intermediate climates such as The Netherlands. In addition to the main focus on thermochromic materials, we will explore the design and proof of concept of coatings or materials that capture light on large surface areas and guide it to a position where it can be used *e.g.* in windows in combination with photovoltaic modules.

Additive Manufacturing research line within the ERP: Although additive manufacturing has already been used in prototyping for many years and, in recent years, also for the production of jigs & fixtures, it is not yet suited for the production of high performance parts with long service time. Partly due to the inherent process conditions and lack of materials specifically developed for the technology, mechanical performance of the 3D printed parts is limited compared to injection molded parts, and not much is known about the long-term performance of these parts. In recent years, a number of fiber reinforced polymer materials have been developed and commercialized to improve this aspect, but the fiber content of these materials is still relatively low, resulting in mechanical properties unsuitable for load bearing applications. As a next step, development has advanced to the use of continuous fiber reinforcement, leading to the development of dedicated continuous fiber printing equipment by companies such as MarkForged. Current state of the art is that this technology can be used with a very limited amount of materials to produce strong 3D parts, but is still inappropriate for structural and validated applications. In order to enable implementation of the technology for aerospace and other components, the range of suitable materials should be extended. In the scope of this ERP we aim to combine our AM expertise with our expertise in polymers and thermoplastic composites, and work together with equipment manufacturers to develop materials and processing strategies for the next generation continuous fiber printing able to produce complex 3D structural parts for long-term use in a cost-effective way.

3. Objectives and approach

Sustainable Buildings research line within the ERP: The objective of this research line is to develop and demonstrate energy efficient and energy generating windows. For energy efficient windows, the focus in on the development of thermochromic coatings, which are directly applied on glass, and thermochromic films. The latter contain thermochromic nanopigments, and are applied to laminate two glass plates *e.g.* for use in safety glazing. To date, thermochromic coatings have been successfully developed within this ERP, and demonstrated on lab scale. Together with commercial partners, this coating is currently being subjected to a series of accelerated ageing tests, and scaled up to pilot scale (1x1 m² windows) to study the techno-economic feasibility and integrate the resulting thermochromic windows in test buildings. Energy performance modeling studies have been executed within this ERP to quantify the energy savings of our thermochromic coatings. They indicated that additional energy savings up to 15% can be feasible for intermediate climates such as The Netherlands.

Currently, the objective of this ERP is to develop thermochromic pigments, both through milling of powders and in a bottom-up chemical synthesis, and integrate them into polymer films for lamination of glass plates and production of safety glass. With these new developed pigments, also the development of additional products like polycarbonate glazing and thermochromic coated polymer films for retrofit applications comes within reach.

In addition to the main focus on thermochromic materials, this research line will explore the design and proof of concept of coatings or materials that capture light on large surface areas and guide it to a position where it can be used in windows in combination with photovoltaic modules.

Additive Manufacturing research line within the ERP: The objective of this research line is to develop materials and processing technologies that will enable the production of complex shaped, (continuous) fiber reinforced products in a cost-effective way. This involves expanding the range of suitable materials, including high temperature polymers, and the impregnation of continuous carbon fiber filaments to ensure good matrix-fiber interaction, as well as developing processing strategies to maximize fiber content and minimize voids in the 3D printed parts. We will implement and validate a materials modelling workflow to predict mechanical performance of 3D printed fiber reinforced parts and to support optimal fiber lay-out and processing strategies for these parts. In addition, we will explore strategies how we can use embedded carbon fibers to achieve additional functionalities, in particular thermal and electromagnetic shielding properties and strain monitoring, relevant for the targeted applications

The current focus of the ERP is twofold:

- to develop suitable processing strategies to achieve high fiber fractions (> 30%), high stiffness (> 40 GPa) and high strength (> 260 MPa) in simple geometries and translate these to complex 3D geometries;
- to develop processing strategies to achieve strain sensing with improved sensitivity and reproducibility.

4. Applications and partnerships

Sustainable Buildings research line within the ERP:

Thermochromic windows existing partnerships along the value/technology chain:

- *Material producers*, such as Kriya Materials, Johnson Matthey and Ferro
- *Polymer film producers*, such as Everlam, Yparex and Sekisui
- *Producers of glass products*, such as Glass GlassforGlass
- *Construction companies*, such as Laudy Bouw
- *End users via housing corporations,* such as Wonen Limburg
- *Hasselt University* (via professorship Pascal Buskens, and PhD student Lavinia Calvi): switching kinetics
- *Zuyd University of Applied Sciences* (via professorship Zeger Vroon, and bachelor students Marco Kong and Romy van Geijn)

Energy producing windows:

- *Solliance:* within this ERP we develop products that are integrated and tested by Solliance
- *Solar window technology companies*, such as Physee

Additive Manufacturing research line within the ERP:

Main applications driving the research line:

- o Complex, lightweight components for aerospace applications, e.g. brackets & hinges
- o Customized, strong parts for sports & leisure applications, e.g. personalized bicycle lugs
- o Structural replacement parts for obsolete components and in remote locations, e.g. in military deployment

Intended partners:

- o *Material producers*, such as DSM, SGL Carbon, Ensinger
- o *Printing equipment manufacturers*, such as Anisoprint, CEAD, Orbital Composites
- o *End users,* such as Fokker, Ministry of Defense, Belgian Cycling Factory
- o *Knowledge institutes,* such as Eindhoven University of Technology, Fraunhofer IMWS

Plan Year 2021

A. Plan – Research Line "Sustainable Buildings"

A.1 Key results so far

Overall goal 2020: preparation of W-doped thermochromic pigments with a switching temperature between 15-25ºC for introduction in coatings and polymer films and sheets for energy efficient glazing.

State of art at start of project: undoped VO_2 powder with switching temperature of 68ºC commercially available; not useful for application in energy efficient glazing.

Key results 2020:

- Successful preparation of undoped and W-doped thermochromic VO_2 powders with adjustable switching temperature at lab scale; 2 patents filed
- Commercially available undoped VO_2 powders successfully milled down in size to pigment particles of ~ 100 nm. Partial loss of functionality during milling (due to crystallinity losses).
- Successful preparation of submicron-sized amorphous VO_2 particles via oxalic acid route, which can be annealed under air to form VO_2 (M); patent filed
- First indications of direct formation of VO_2 (M) via oxalic acid route, without need for thermal anneal.
- Two scientific publications on 'quantification of the energy performance of thermochromic windows' and one on 'switching kinetics of thermochromic windows'.

A.2 Key objectives and expected results

Overall goal 2021: Preparation of A4-sized energy efficient window with pigmented PVB film as thermochromic interlayer

Expected essential results 2021:

- Optimized pigment production processes (both top-down via milling, and bottom-up via chemical synthesis);
- Successful integration of thermochromic pigments in PVB polymer films (lab scale) with retention of thermochromic properties;
- First A4 sized demonstrator of energy efficient window with pigmented PVB film as thermochromic interlayer;
- At least 1 new patent application and 2 scientific publications.

B. Plan – Research Line "Additive Manufacturing"

B.1 Key results so far

Overall goal 2020: development of suitable processing strategies to achieve:

(1) high fiber fractions (> 30%), high stiffness (> 40 GPa) and high strength (> 260 MPa), and

(2) strain sensing with improved sensitivity and reproducibility

State of art at start of project: initial 3D printed parts with 10-20% carbon fiber, 10-15 GPa stiffness and 150-190 MPa strength and initial proof of concept for integrated (qualitative) strain sensing

Key results 2020:

- Proof of concept of mechanical strength (500-600 MPa) and stiffness (39-42 GPa) in simple test geometries

- Report comparing the economics of producing fiber-reinforced 3D printed parts with metal parts or composites parts produced by other methods (*in progress*)
- Implementation of developed processing strategies in complex 3D demonstrator, i.e. fiber reinforced bicycle components
- Implementation of modelling workflow for continuous fiber AM
- Demonstrator of integrated strain monitoring at multiple locations in the project
- 1 patent application regarding integrated strain monitoring with improved sensitivity, and 1 patent application regarding particle alignment during printing

B.2 Key objectives and expected results

Overall goal 2021: development of material and processing strategies to obtain thermal properties suitable for high performance (aerospace) application, i.e. thermal stability (> 125°C) and stability in thermal cycling (-50°C to 125°C)

Expected essential results 2021:

- 3D products of high temperature polymers (PEKK/PEEK) in combination with continuous fiber, optimization of adhesion matrix and fiber and between matrix layers
- Failure mechanisms correlated with microstructure, development of material and processing conditions to optimize performance under compressive and cyclic loading
- Integrating thermal performance (thermal conductivity, resistance against thermal cycling) for high mechanical performance parts
- At least 1 new patent application and 1 scientific publication

Figure 2: 3D printed parts with continuous carbon fiber

i-Botics

ERP Contacts: H. Young (Project Lead), J. van Erp (Lead Scientist), H.-J. van Veen (Science Director)

Program description

1. Problem definition

Our society increasingly encounters robots at the workplace and at home, which often function with a high degree of autonomy, particularly when task variability is low and the task environment is well controlled and separated from locations were humans are allowed. However, for performing operations in ever-changing situations with unpredictable task constraints and demands, high degrees of cognitive, perceptual, and motor skill intelligence and flexibility are required at a level not yet delivered by autonomous robots. Human control is vital in these conditions. Robot intelligence plays an important role when implementing robots in conditions in which part of the tasks could be done autonomously and others with human control. Distributing tasks between the human and the robot optimizes operational performance, yielding a more economical solution that is pleasant to work with. Such solutions are strongly intertwined in i-Botics, even in full user-in-the-loop solutions.

Examples of relevant environments for i-Botics include rescue situations, strenuous inspection and maintenance (e.g. subsea), work at construction sites, and operational logistics. In these situations, hybrid solutions between people and robots are emerging, though various technological challenges have not been adequately dealt with. Often, these unsolved challenges stand in the way of a truly effective, productive, flexible, worker-friendly, healthy and safe human-robot interaction. i-Botics focuses on optimal human-robot interaction in two challenging, unpredictable and dynamic situations: human-controlled robots for e.g. installation, inspection, maintenance, repair and emergency response; and wearable robots for human enhancement in rehabilitation and heavy work environments.

2. Positioning

Successful human-robot teaming requires expertise in many different fields: human perception and cognition, sensor technologies, Artificial Intelligence (AI) and system integration. TNO's researchers are considered top of their fields in the necessary expertise, but even more importantly: TNO is well-equipped to make multi-disciplinary solutions actually work. Currently, i-Botics leads a consortium in the ANA Avatar XPRIZE, a world-wide benchmark competition on transporting human presence to a remote location in real time. Of the 77 teams from around the world, Team i-Botics is emerging as a serious finals contender.

The three ERP i-Botics research lines and their positioning are:

<u>Remote, dexterous (bi-)manipulation</u>: Systems mainly focus on controlling a single robot arm with a simple gripper using complex interfaces with limited "transparency" such as joysticks and game controllers. The state of the art in dexterous manipulation is restricted to the development and use of only a few advanced robotic hands, such as Shadow Robotics Hand, Prensilia IH2, the Pisa Softhand, and NASA's Robonaut Hand. A looming unsolved challenge is the intuitive control of these complex hands and providing adequate haptic feedback on arms, hands, and fingers. Based on both robotic engineering expertise, human manual control and haptic perception expertise, TNO uniquely combines dexterous robot arms and hands (obtained from external partners) with intuitive hand and finger tracking and haptic feedback.

<u>Visually enhanced telepresence</u>: Current teleoperation technology suffers from an eminent risk of data overload and degradation (e.g. caused by delays). Advanced algorithms for data selection and conversion into actionable intelligence, for either human or robot, can mitigate this risk. i-Botics goes beyond simple vision-based automation and works towards a full 3D telepresence approach through VR-mediated control. Very few organizations are working on this state of the art approach; these include DORA (University of Pennsylvania), Guardian GT (Sarcos Robotics), HERMES and CSAIL (both MIT), NASA and ESA, DexROV (ROV consortium), NEDO and TELUBee systems (Keio University). TNO has developed world-leading virtual/augmented reality applications that enable e.g. maintenance operations, operator or robot training, complex navigation using Simultaneous Localization and Mapping (SLAM) and advanced automatic environment recognition (e.g. for data reduction).

<u>Wearable robotics:</u> Various passive exo*skeletons*, for e.g. trunk or arm/shoulder support, exist. Some are close-to-market-application products: lightweight and relatively easy to use. However, their effectiveness has been proven only for static work postures and their adaptability to multiple tasks is minimal. Active exoskeletons are potentially more adaptive, though they need to be made more effective for realistic tasks (not only for isolated movements), thus making them more attractive for industry. The development of exo*suits* is further away from industrial application; for rehabilitation purposes, Harvard University is world leading. TNO plays a role in the

development and evaluation of various passive and active exoskeletons (e.g. RoboMate, Exobuddy, Skelex, Laevo, and Spexor) and brings well-recognized expertise on human-exoskeleton interaction, i.e. biomechanics, anatomical fit, sensing human intention and control, comfort and acceptance, and industrial implementation.

3. Objectives and approach

Multi-year ambition is to optimize human-robot collaboration to conduct various tasks in the most challenging, unpredictable and dynamic situations. The focus aligns with the ANA Avatar XPRIZE, and is on robotic systems to transport human senses, skills and cognition to a remote environment in real time to enable us to see, hear, touch and interact with physical environments and other people. Additionally, the focus is on wearable robotic systems to provide mechanical support to workers in physically heavy, mobile, and 'difficult-to-automate' situations. ERP i-Botics funds two PhD positions: Ali Tabasi (VU) woriking on exoskeletons (WP3) and Sara Falcone (UTwente) working on embodiment and teleoperation (WP1/2). i-Botics collaborates with the ERP Appl.AI on several topics, actively sharing knowledge, technology and experts.

WP1: Bimanual manipulation and agency & ownership (i-Shield)

Objective: To realize intuitive, bimanual dexterous remote control.

Relation with Roadmap: All TNO roadmaps that involve robotic systems with diverse tasks, unpredictable environments and in which the stakes for (un)successful operation are high: Information & Sensor Systems, National Security, Operations & Human Factors, Biomedical Health, Space & Scientific Instrumentation, Maritime and Offshore.

Approach: If a robotic system's tasks are diverse, the environments unpredictable and the stakes high, robots continue to rely on human involvement to carry out tasks. The common solution in these cases is teleoperation. Within WP1 we aim to develop a state-of-the-art bimanual teleoperated set-up, including intuitive control and end-effectors for dexterous manipulation, tele-sensing and rendering in the form of haptic feedback and other critical touch cues. We advocate that embodiment of a remote manipulator may improve dexterous performance in tele-robotics. This warrants further testing of embodiment in tele-robotics to gain knowledge on the most important parameters that enhance performance through embodiment of robotic systems.

WP2: Visually enhanced control

Objective: Developing adaptive, co-active, vision-based control of a robotic system in complex, unknown environments.

Relation with Roadmap: Information & Sensor Systems, National Security, Operations & Human Factors, Health Technology & Digital Health, Networked Information, Maritime and Offshore, *possible future roadmap:* Smart Industry.

Approach: The past years we developed technology for 1) multi-sensor integration from a robotic platform to an operator using VR, 2) minimizing latency using data selection and optimal streaming, 3) 3D environment reconstruction and understanding. This technology includes incorporation of various AI algorithms, systematic engineering of suitable sensor suites and a modular software framework for acquisition, processing and visualization. The approach for 2021 is to optimize and evaluate the complete pipeline for subsea inspection and maintenance tasks (through H2020 project IFESTOS). To achieve this optimization, more fundamental work needs to be done concerning point 3) - extending the work done in 2020, in which 'multi-sensor - multi-agent' SLAM was developed, as well as a hybrid AI approach for environment understanding.

WP3: Exoskeleton/wearable robotics

Objective: To develop knowledge and technology for a wearable robot to provide mechanical support to workers involved in physically heavy, mobile, and 'difficult-to-automate' situations.

Relation with Roadmap: Health Technology & Digital Health, Biomedical Health, Work, Operations & Human Factors, Maritime and Offshore, Buildings & Infrastructure.

Approach: Focus on exoskeletons around industrial task requirements. To this end, we focus on finding optimal control algorithms that minimize complexity while increasing performance. We will identify a set of input variables that is practical yet effective. Finally, we asses human body impact of exoskeletons in both lab and industrial settings.

4. Applications and partnerships

Maritime and Offshore; Robotics for underwater operations. Remote inspection and maintenance of marine infrastructure - such as quay walls, jetties, offshore (wind) structures, cables and pipelines - are important applications of i-Botics technology. Operations in marine environments are expensive and complex. Obtaining enhanced Situational Awareness and Intuitive control will ease operations thereby saving costs and enlarging the window of operations. With the (JIC) i-Botics underwater robotic program line that heavily relies on ERP i-Botics developments, we have focused on building a blended reality environment with multi-sensory input – a crucial step in numerous underwater applications. The JIC program has a flexible approach which enables partners to influence the goals of the program. The program is highly appreciated by the industry, with 15 partners and growing.

Key stakeholders: Boskalis, Rijkswaterstaat, DEME, Van Oord, Shell, Equinor and various technology providers.

Maritime, Offshore and Renewable Energy; Robotics in dry environments. For operation of cranes on ships, robotic arms and manipulators for maintenance in offshore wind turbines (Nacelles), and for robots on offshore platforms, the developments of WP1 and WP2 add significant value. By reducing the number of persons, offshore safety is increased and costs are reduced. Especially reducing the need for people to go offshore hugely impacts the entire industry. WP3 creates large added value in ship building and maintenance, where there are heavy workloads and repetitive tasks in complex environments. Our wearable robotics achievements help implement COTS exoskeletons and develop new technologies to optimize implementation of wearable robotic systems. Linked to the ERP, i-Botics has been awarded multiple projects in this domain in which technologies for intuitive robotic arms, cranes and wearable robotics are being developed in collaboration with industry.

Key stakeholders: Cargotec, MacGregor, Damen, Fincantieri, IHC, Navantia, SkelEx, Shell, Equinor, Orsted, SPRINT Robotics, Sintef, AnyBotics and ETH.

National Security. The National Security domain has a number of important stakeholders and applications, for which the advances in all work packages are highly beneficial. Many jobs in this domain can be dangerous, and thus desirable to robotize. WP1 and WP2 develop the crucial technologies to control robotic systems intuitively and with the required information from the changing environment. Physical workload for specific jobs in this domain can also be high, due to specific gear and repetitive movement, e.g. for ME (mobiele eenheid) when using shields. WP3 provides the required innovations to introduce this technology. i-Botics is currently carrying out an explorative project to identify the most stringent and high impact applications for robotic technologies in the National Security domain. This project involves many stakeholders and will be followed by a multi-year R&D program.

Key stakeholders: Politie, KMAR, DJI, DSI, Fire Brigades, Satefy organizations, Security companies, Urban Search And Rescue teams, MinJenV.

Healthcare. The COVID-19 crisis has shown how desirable remote care can be. More generally, remote care enables (scarce) expertise at a distance and scalability. Since in almost all applications in this sector the robotic systems interact with human beings, tedious operation, real-time situation awareness and social interaction are extremely important. WP1 and WP2 provide technology to facilitate these processes. In addition, wearable robotic systems, researched in WP3, are of great use in the healthcare, in which physical workload can be very high as a result of lifting people and the adoption of undesirable postures. On the ‘cure’ side, surgeons who are experts in robot-assisted endoscopic surgery are able to ‘tele-mentor’ less experienced surgeons all over the globe, using i-Botics technology.

Key stakeholders: SkelEx, Laevo, Roessingh Centrum voor Revalidatie, OttoBock, Haption, Halodi, UVA.

Defense. For the Royal Netherlands Army remote controlled robotic systems are becoming increasingly important. A separate entity, comparable to a brigade staff (RAS Unit, part of 13th Brigade), was created to explore and develop the implementation of robotics and AI within the Dutch army. TNO / i-Botics work closely together with this unit. The joint concept development and experimentation has a strong relation to technological developments of WP2 and Appl.AI (SNOW, MMT-MHC). For physical human enhancement, the developments in WP3 related to wearable robotics are of significant added value. The Royal Netherlands Navy uses underwater robotics which benefit from developments in WP2 and WP1, specifically for Mine Counter Measures. Additionally, WP3 links to the maintenance activities for Navy vessels. Lastly, WP2 developments are included in a feasibility study for the Royal Netherlands Marine Corps.

Key stakeholders: Royal Netherlands Army, Royal Netherlands Navy and specifically RNLMARNS, KMAR, RAS Unit, MinDef and EODD.

Plan Year 2021

A. Plan – Research Line “Bimanual manipulation and agency & ownership”

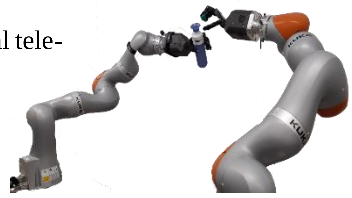
A.1 Key results so far

- Role of haptic feedback and substitute haptic feedback in dexterous tele-operation (Eurohaptics paper). The results reveal that participants prefer to have haptic feedback in tele-operation, although their performance in the tele-operated box and blocks task did not improve.

- Position paper on the role of embodiment in tele-operation, set of guidelines to apply embodiment in telerobotics and identification of important research topics (Frontiers in Robotics and AI paper).
- Realization of a bimanual set-up, including two arms, hands and advanced force-sensors for haptic feedback. Only the most prominent R&D institutes start to explore advanced techniques such as wireless arm and hand tracking and employing robotic arms as input device to control dexterous manipulator, such as the Shadowhand.

A.2 Key objectives and expected results

- Improved haptic feedback through the sensing and rendering of pressure, low frequency vibration, high frequency vibration, temperature, indentation, skin stretch, force, limb position and/or displacement.
- Knowledge on bi-manual control.
- Ultimate embodiment experiment to optimize parameters that enhance embodiment and increase intuitive control.
- Extending the current TNO unimanual task battery for dexterous bimanual tele-operation performance to benchmark system performance.
- All points above use and contribute to a state-of-the-art bimanual tele-operation set-up.



B. Plan – Research Line "Visually enhanced control"

B.1 Key results so far

- Publications at IEEE IROS and HCI, 2 other publications will be submitted (end 2020), showing that full visual information improves operator task performance, and that our information selection approach is useful for incremental co-learning (of robot and operator).
- Exploitation of developed visually enhanced control model and software in projects SURE, ANA Xprize AVATAR, H2020 MOSES, ERP AI - SNOW and some smaller projects (e.g. 'TKI Dakplaatrobot').
- Successful graduation of seven students with i-Botics related assignments (in collaboration with UTwente, TU Delft and UvA).
- A NENnovation Student Award for using a NEN norm in our experiment on the effect of visual cues for robotic task performance (see also the HCI paper).
- Invited presentations at (inter)national conferences such as the Mathworks Research Summit and the Robotics+Vision beurs (Mikrocentrum).
- Multiple demonstrators of developed technology; used to show to potential customers, colleagues, collaborators and other stakeholders.

B.2 Key objectives and expected results

- Integrated visual control pipeline and method for tuning the complete pipeline/platform.
- Method/model for visual scene understanding in a robotic context; estimate interaction possibilities with a large variety of perceived objects using a hybrid AI approach. The ambition is to test this method/model through a use case with a link to IFESTOS. We also co-formulated a student assignment with the ERP AI – SNOW.
- Publication (paper/report) on pipeline performance.
- Publication (paper/report) on method for visual scene understanding.
- Movie (or other demonstration) of complete pipeline.

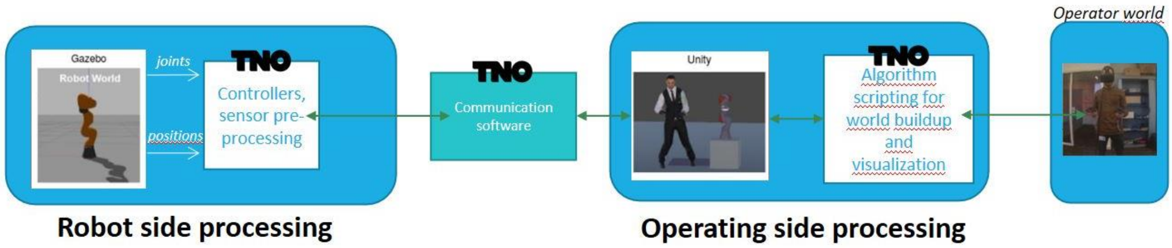


Figure 1 Overview of developed visually enhanced control pipeline.

C. Plan – Research Line "Exoskeleton/wearable robotics"

C.1 Key results so far

- Systematic reviews showed that readily available arm support exoskeletons only come with passive support and are not validated in working environments, and that active exoskeletons only exist for back- and low-back support (paper in J. Ergonomics).

- Comparisons of different algorithms (kinematic-drive, fore-arm EMG-driven, and a hybrid control-mechanism - paper journal Biomech).
- Validation that back muscle activation has to be an input variable to improve the accommodation to the consecutive phases in the lifting movement.
- A simulation environment in OpenSim, which can be used to model joint reaction forces and actuators for working with an exoskeleton.
- Validation that posture largely effected total torque and torque generated by the exoskeleton (paper IISE Trans. Occup. Ergon. Hum. Factors). Active actuation of the exoskeleton may help widen the field of exoskeleton applications (towards a larger range of postures).
- Experiment with plasterers (highly dynamic work). Muscle activity as well as perceived exertion were reduced when working with the exoskeleton (paper submitted).

C.2 Key objectives and expected results

- Find the optimal sets of inputs and control algorithms for minimizing the mechanical loads on the human body. A proper control strategy should detect fatigue and account for changes in input variables (i.e., the muscular activity and body kinematic change as function of fatigue).
- Test and improve our sensor-based motion analysis tool to advise on exoskeleton selection.
- Develop a demonstrator with an active back support exoskeleton in collaboration with IIT, to experience the different control variables and algorithms.
- Develop and test a smart, fully mobile calibration procedure for an active back support exoskeleton. The currently suggested calibration procedure requires lab settings and equipment, which may not be available in the workplace thus leading to suboptimal support from the exoskeleton.

HybridAI

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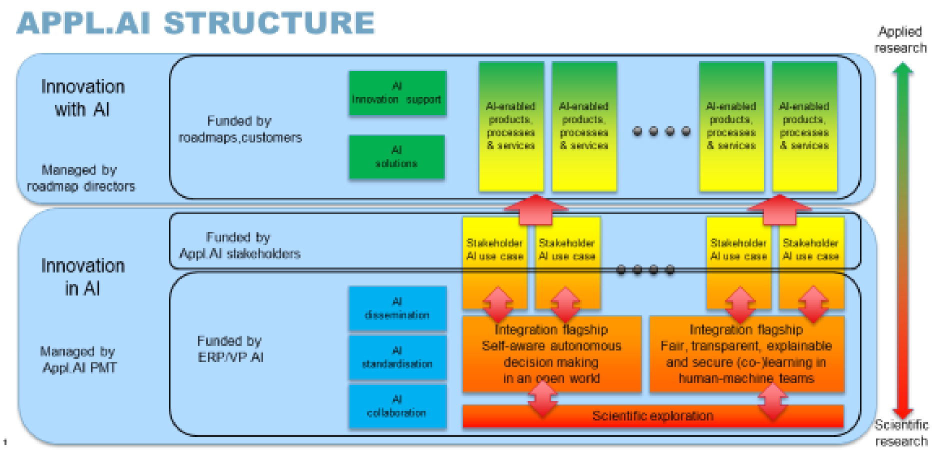
Program description

1. Problem definition

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 done 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. Our ambition is to build on an already strong position and accelerate AI innovation through focus on integrational aspects of AI.

2. Positioning

AI has really taken center stage as the key enabling technology for approaching virtually any problem in the world. Because of this enormous impact, the leading corporates (e.g. Uber, Google, Amazon) and academic/research institutions (e.g. MIT, Stanford, Oxford) have invested heavily in developments in 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 so that all central activities with respect to AI are aligned into one program. 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 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 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 achieve a recognized position on the system integration and architecture level for AI applications.

3. Objectives and approach

The long-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 units with AI as important enabler, we conclude that it 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.

The program is structured in generic research within the two integration flagships, and application centered research in use case projects that support and strengthen each other mutually. Commitment of external stakeholders in the uses cases shows their needs and is expressed through a multiplier on the research funds.

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 topics are key for future AI applications in domains such as Health, Mobility, FinTech, Labor/Recruitment, Energy, Justice, Security, and Defense:

The objectives of the *SNOW flagship* project are to develop, integrate, demonstrate and evaluate Al 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.

The aim 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 (subject) data sources and communicates its fair advices geared towards phenomenon researchers, consultants and subjects.

Both SNOW and FATE employ Hybrid AI by combining data-driven and knowledge-driven approaches to 1) enable effective modeling of the physical world and the ethical and legal conditions under all circumstances, and 2) allow for context-sensitive and personalized explanations of the decision processes.

To unify the flagships in an overall program ambition, we are currently defining an Appl.AI Moonshot. This will strengthen our focus and communication within and outside TNO.

4. Applications and partnerships

Applications, partnerships and collaborations are three main drivers for the Appl.AI program. There are two work packages dedicated to applications and partnerships: scientific exploration and (inter) national collaboration. The program has three different advisory boards: a scientific advisory board, the Appl.AI Community and an advisory board with stakeholders from the different Dutch ministries of the Taakgroep TNO. In addition, we implement collaborations with external partners such as CBS and Fraunhofer.

Academic collaborations are developed and extended in the Scientific Exploration work package. The objective of this work package is to research concepts, methods and techniques that are needed to achieve the long-term Appl.AI goals. The work package will mostly deliver research papers and fundamental knowledge. The activities are primarily conducted by (associate) professors and PhD researchers. There are currently seven (associate) professors and six PhD students (partly) funded by the Appl.AI program. Several PhD projects are partly funded by two NWO research programs: Efficient Deep Learning and Smart Connected Bikes.

The objective of the (inter)national collaborations project is to identify, setup and work in national and international collaborations. This includes both direct collaboration with peer institutes and working in ecosystems. Through the program in general and this project in particular we want to position TNO as one of the top players in the AI field. We have initiated a joint project with Fraunhofer IOSB on "Value-oriented Design and Enforcement for Responsible Automated Decision Making" and cooperating with the University of Amsterdam and CWI on Meaningful Control of Autonomous Systems (MCAS). We are pursuing a collaboration with the University of Twente within the i-Botics context and participate in an early adopter program instigated by Boston Dynamics for their Spot quadruped robot. Within the Netherlands we work together with partners in the NL-AI Coalition and the NWA. In Europe we are part of the CLAIRE initiative and are partner within the Big Data Value Association (BDVA). We are part of the H2020 projects VISION and TAILOR which aim to build European networks of excellence in AI. Furthermore, we work on standards for AI at the national (NEN) and international level (CLAIRE, BDVA) by participating in working groups. More information is given below.

Professors and associate professors	Universiteit Leiden The Netherlands, Maastricht University, TU Delft, liacs, TU/e, Radboud Universiteit
PhD students	VUB Vrije Universiteit Brussel, Universiteit Utrecht, TU Delft, Universiteit van Amsterdam, TU/e
Collaboration	NEN, CLAIRE, NL AI Coalitie, GRAKN.AI, Fraunhofer IOSB, Hybrid Intelligence, Universiteit van Amsterdam, NWO, EDL, BDV Big Data Value Association, nationale wetenschaps agenda, cwi, cbs
Use cases	Ministerie van Defensie, ECSEL Joint Undertaking, kpn, SMITZH, Strukton, ARCADIS, cbs

Plan Year 2021

In this chapter the results of 2020 and the plan for 2021 are described. In section A the overall program is presented, in section B and C the flagships SNOW and FATE and their associated use cases, respectively.

A Plan – Appl.AI program

A.1 Key results so far

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. We expect that the AI proposition of TNO will further improve in 2021 as we now articulate what we especially need from new use case proposals through the definition of research white spots for the two flagships.

Key results on program level for 2020 include

- contribution to 2 bln national Groeifonds proposal 2021-2027 NL AIC with 70mln ask for TNO funding
- commitment of 3 mln SMO funding by EZK for NL AIC for data sharing and other topics, which will be funneled through TNO/Appl.AI.
- position paper on Appl.AI research goals at the TAILOR workshop of the ECAI2020 conference
- white paper on Appl.AI goals and plans
- TNO AI strategy development with input from all units
- Communication:
  - general Appl.AI Business Development presentation and event
  - website - on average 4000 visitors of the webpage per month and 75 clicks for contact information, which has resulted in multiple new leads for TNO such as Airbus, Demcon, Ministry of Social Affairs, Inspectorate of Social Affairs, WRR, and Municipalities
  - webinars – e.g. webinar AI for public domain with 150 visitors
  - monthly newsletter r– 150 members
- virtual AI lab to facilitate internal collaboration and external presentation of results
- embedding of TNO AI in various national and international communities
- joint AI project with Fraunhofer IOSB
- new Appl.AI communities: TNO AI community (incl. new Appl.AI Unit Meetings), scientific advisory board, Appl.AI Community, TNO Taakgroep klankbord
- partner in multiple EU proposals: VISION and TAILOR granted, PRE-TERM and CO-OPERA submitted.

A.2 Key objectives and expected results

The key objectives for 2021 are

- improved research alignment between flagships and use cases
- strengthening the TNO AI community including involvement of all units
- positioning the TNO AI research and propositions in the outside world

Expected results on program level for 2021 are:

- by active engagement with NL AIC and its eco-system, we guard the funding of TNO AI through the Groeiplan and other relevant funding bodies such as at NWO, at the EU etc. Amount and instruments are to be established. If granted, we should at least add 5 mln to TNO's AI funding in 2021. This budget is assigned for higher TRL research together with partners.
- data sharing initiative in NL AIC with funding from EZK embedded in Appl.AI. In 2021, this will lead to an added 1,5 mln euro funding (ex.co-funding from relevant sectors) which will be partly shared with partners.
- position paper of the Appl.AI Moonshot
- implementation of the TNO AI strategy with all relevant units
- communication: 1 TNO event, regular updates website, 6 webinars, a virtual lab, and a monthly newsletter
- profiling of TNO AI in different national and international communities
- developing partnerships with Fraunhofer, CBS and i-Botics and exploration of other potential partnerships
- further development and mutual value out of different communities: scientific advisory board, Appl.AI community, TNO Taakgroep Klankbord
- multiple EU proposals submitted and granted.

B. Plan – Flagship SNOW: Safe autonomous system in an open world

B.1 Key results so far

The focus in 2020 for the flagship SNOW is on the characterization of novel objects, context-aware planning, and characterization of own competencies. We developed real-time hybrid AI software that integrates machine learning, a knowledge graph and symbolic reasoning on a quadruped robot to detect and characterize (novel) objects, assess own competencies, and plan a course of action based on the context and operator commands. For research and testing we developed a search and rescue scenario with Key Performance Indicators (KPIs). The KPIs of the autonomous system in this experiment include the operational effectiveness, the number of operator interventions during the experiment, and the complexity of the operational environment. The aim of the experiment to be conducted at the end of 2020 is to demonstrate that the hybrid AI software can reduce the number of operator interventions during a search and rescue task with respect to a remotely controlled robot while maintaining the same operational effectiveness.

In the SNOW flagship project, we developed algorithms for the detection and characterization of novel objects based on a taxonomy, for context-aware planning, for representation of interacting user preferences and for characterizing own performance in the current operational conditions. Next to that we developed an ontology that represents the hierarchical structure of the hybrid AI software components.

The use cases associated with the SNOW flagship project in 2020 are:

- Meaningful human control: 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.
- Truck platooning: AI algorithms for situational awareness in automated driving in truck platoons.
- FAIM: AI algorithms for resource management in mobile communications networks.

In 2020, Fraunhofer IOSB committed itself to a joint project with TNO on "Value-oriented Design and Enforcement for Responsible Automated Decision Making". This project, which aligns with the elicitation of user preferences in the SNOW project, has a duration of 3 years and a budget of 1 M€ for each partner. The NL MOD KIXS department made available three trainees in 2020 for research on the translation of user preferences to a course of action.

B.2 Key objectives and expected results in 2021

The high-level objectives of the SNOW flagship project remain the same as in 2020. The focus in 2021 is on improving autonomy, i.e. reducing the number of operator interventions with respect to 2020 by eliciting operator preferences, understanding interactions between objects in the environment, and an assessment of own competencies.

Expected results in 2021 are:

- Improved real-time hybrid AI software for a quadruped robot that enables 2 times fewer operator interventions in the search and rescue experiment than in 2020 at the same operational effectiveness and complexity of the environment.
- An algorithm for context and task dependent reasoning about novel objects and (dynamic) relations in the environment.

- A method and algorithm for eliciting operator preferences and risk-based planning
- An algorithm for understanding own competencies in novel situations
- At least four articles on the research described above.

Recognized research white spots that will be handled in newly defined use case projects and are highly relevant for awareness of the situation, the user, and own competencies (self-awareness) include:

- Characterization of operational context and anomalous behavior (situation awareness)
- Calibrated classifier (situation and self-awareness)
- Elicitation of uncertain or missing user preferences (user awareness)

New partnerships and follow-ups that are planned for 2021 include cooperation with the University of Twente in the scope of the i-Botics innovation hub for research, development, and implementation of interaction robotics and cooperation with the Brightsite program on robotics for inspection of chemical plants.

C. Plan – Flagship FATE: Responsible human machine teaming in a dynamic world

C.1 Key results so far

In the FATE flagship the aim is to develop an expert assistant for sensitive domains, where the learning data needs to be handled with care and the user needs to be addressed focused to her role: researcher, consultant, subject. In sensitive domains confidentiality, bias and fairness are key aspects. While the expert assistant is functional the environment may change, partially as a result of the system. Two results guide the FATE flagship as a whole and its connected use cases. First we developed an initial *generic architecture* in order to map the use cases to this architecture. Second, we developed KPIs for the key research directions: fairness, secure learning, explainability and co-learning.

On the topic of ***fairness,*** we designed definitions of relevant types of fairness and biases from legal, ethical and policy perspective. We also developed algorithms for bias detection, explanation and mitigation. These algorithms are applied in different use cases. In the Diabetes-2 use case and the skills matching use cases biases based on age, gender, and ethnicity are detected and quantified. In the AI4Justice use case effects of self-fulfilling prophecy are detected and mitigated for high impact justice applications.

For learning from confidential data, we developed specific ***secure federated learning*** algorithms, that were also applied in real-life cases in the Oncology, the Diabetes-2 and the Money Laundering use cases.

For ***explainability*** we developed algorithms for single, personalized AI generated explanations that can be used for the roles of a consultant (e.g. a doctor) or subject (e.g. a patient) to understand the individual decisions of the AI system. The focus is on understanding and trust calibration. Next to that we developed adaptive techniques for adjusting the system behavior (the recommendations and the type of explanations) to human’s behavior, interaction design patterns, a first version of a user model (Theory of Mind), and evaluation methods for the context-sensitive personalized explanations.

Application of hybrid AI solutions are shown in the use cases Smart Buildings, Think or Sink and Carefree. The challenge of combining physical models and data-driven machine learning is addressed, with aspects of explainability and fairness.

C.2 Key objectives and expected results

In 2021 FATE will focus on 1) ***enforcing fairness*** by controlling biases depending on the legal, ethical and policy conditions for different learning scenarios: controlling bias either as pre-, in- or post-processing step, 2) harmonized ***explanations*** for multiple roles, and 3) adaptivity of AI systems to systemic changes in a group of users, such as trends in society.

Expected results in 2021

- Controlling bias and enforcing fairness in the respective learning phases, pre-/in-/post-processing
- A comparison of possibilities and limitations between bias controlling measures
- Detection of systemic changes
- Explanations of outputs in relation to the social context and history of explanations
- Scalability studies for secure federated learning in number of parties, features and samples
- At least four articles on the research described above.

The following recognized research white spots will be handled in newly defined use cases:

- Explaining the output of the AI-model to the human for appropriate understanding and trust calibration.
- Controlling bias as post-processing step
- Bias detection and mitigation in other scenario’s than class prediction, such as: regression, data scaling,

missing value imputation, outlier detection, and language modeling.

- Secure federated learning for other problems than class prediction, such as: regression, data scaling, missing value imputation, outlier detection, and language modeling.
- Detection and mitigation of systemic influence of the operational system.
- Methods for handling the changes/drift in the population/data
- Methods to enforce that learning is in line with the initial goal of the system

D. Summary & outlook

The Appl.AI program has expanded its impact in research, strategy, visibility in and outside TNO in the first year. Appl.AI yields research results that are in the frontline of the needs according to the EU AI research agenda. The TNO strategy has been aligned with the Appl.AI AI strategy initiatives. In the NL AI coalition Appl.AI is a recognized brand with a devoted role in the management of part of the NL AIC data sharing budget. With the sharpening of our research focus, the establishing of advisory boards, and building on the results of 2020, expectations are high on the way to the Appl.AI Moonshot.

Exposense

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Program description

The aim of the program is to deliver comprehensive equipment and models for the management of the impact of particulate matter (PM) exposure on air pollution-related human health. To this aim two important aspects are foreseen. First development of portable sensors (< 25 x 25 x 25 mm^3) and second an integrated model for the assessment and management of PM exposure. Both will be combined in system demonstrators and proof on concept setups. In a later stage the PM sensor and models will be complemented with other modalities for Volatile Organic Compounds (VOC) such as benzene and formaldehyde, which are on the list of substance of very high concern (SVHC). The technology developments and knowledge breakthroughs described in this document are needed to achieve personalized assessment of external exposures, with a high resolution in time and space and in real time.

1. Problem definition

Our health is impacted by the environment we live in, consisting of a combination of exposures (e.g. lifestyle factors, chemical exposures, social interactions and stress). While the genome is mapped it is believed that only ca. 20% of the burden of disease are explained by it. Therefore the concept 'exposome' – the total of exposures a person experiences during a lifetime – will help to close this gap in knowledge. Moreover, better understanding of how exposures are related to disease will enable the development of effective personalized preventive measures in this area.

Exposure to airborne particulate matter (PM) is responsible for about 4% of the disease burden in the Netherlands and an additional 4 – 5% are due to work-related exposures. Air pollution therefore is one of the most important risk factors, in the same order of magnitude as overweight (5%)[1]. 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 first application domains of the technology will be occupational health and public respiratory health.

2. Positioning

There are several sensors and sensor systems which are portable and can detect PM and other air quality parameters. The RIVM keeps a good overview on some of the most used apparatus (https://www.samenmetenaanluchtkwaliteit.nl/apparaten-en-kits). At the same time there are several studies, which indicate, that these kind of portable sensors can be used to follow trends, but are not reliable enough to be used to indicate limit values. The error margins and the device to device matching is usually too big, making results gathered with the same type of sensor at different times or locations very difficult to compare.. Furthermore none of the devices has a chemical identification for PM sensing. We developed a unique TNO position which has been protected in 3 patent applications (2019 – 2020).

For the occupational domain, sensor based exposure assessment and modelling is in its infancy. Although sensors are commonly used at workplaces to detect very acute toxic compounds stationary, not much experience is published on using mobile sensors for personal exposure. The models currently used to estimate worker exposure give task or day averages mostly based on source-receptor approaches. Only few publications are available that describe dispersion model like approaches based on sensor networks. TNO is one of the international leading institutions in this domain.

Air quality assessment is for regulatory compliance performed at annual level. This time resolution is not useful to assess personal exposure in relation to disease. A rough grid of measurements stations is available in the Netherlands providing (in many cases) hourly measurements for common air pollutants (LML-network). Models

[1] https://www.gezondheidsraad.nl/documenten/adviezen/2018/01/23/gezondheidswinst-door-schonere-lucht

are available to estimate concentration levels in hourly resolution from these LML stations. However, the spatial resolution is still not detailed enough to be useful for personal exposure assessment. TNO owns models that can increase the resolution in place. Many initiatives of civilian participation in assessing air quality are currently popping up, varying from citizen science project like 'samen meten', to bicycle and Google projects of IRAS. By these initiatives the air pollution becomes visible in real time. The challenge is how to use these sensor data to generate in combination with models trustworthy predictions of concentrations of pollutants in air for a coming time period. TNO's ambition is to grab a unique position in this domain, by combining models and sensor data to predict air concentrations and to use the models for source apportioning.

TNO has shown that mobile data can be linked to stationary measurement data (NWA start impulse, measurement during Nijmegen 4 daagse 2019). Furthermore TNO has been able to couple the global emission models of LOTOS – EUROS to local information gathered by SUMS models (ERP results 2019/2020). In doing so data with a lot better spatial resolution could be gathered. (from 7km x 7km to under 1km x 1km).

In order to bring models and sensor data together a data infrastructure is needed to store, combine/synchronize and analyze the data and automate the translation of sensor data into useful and understandable information, which can be provided as feedback through apps or dashboards.

3. Objectives and approach

Sensor development for PM and VOC exposures: Low cost and portable PM sensors are currently available. However, they suffer from major drawbacks: 1) both the detection limit and reproducibility are in general poor, and 2) they only can assess mass or size of the particles. To make a significant step to correlate particulate matter to effects on health, it is important to know the chemical composition of the particles. The proposed technology breakthrough is to discriminate the size of the particles (i.e. 2.5um /4 um / >10um diameter) in a low cost (<2000EUR) and small size solution – as well to chemically identify PM with respect to both organic and inorganic components. Concentrations of PM which have to be measured are in the range between >10mg/m3 to 25□g/m^3 to be in agreement with the European Air Quality standard[2]. In parallel a platform for adding VOC's to the sensor will be developed to be able to measure those gases at a level <20 ppb (benzene) and <100ppb (formaldehyde).

Analysis and interpretation of external sensor data and integration with models (external exposome): Currently air quality and occupational exposure are being modelled completely independently from each other and for very different purposes. The resolution in time and space is low (often 8 hour time weighted average for occupational exposure and mostly annual averages for environmental exposure) and the predictive power for personal exposure levels is limited. Therefore exposure assessment can only be done at group level and in a time integrated manner. We aim to predict exposures at the personal level, being able to identify differences between individuals and within individuals over a (working) day. A higher resolution of exposure assessment methods in time (1-5 minutes) and space (1-10 meters) is needed to increase the predictive power to the individual level. Breakthroughs aimed for in this ERP include improvement of time and spatial resolution of exposure models, methodology for data fusion with sensor data (challenges: difference in resolution and dealing with uncertainty) to increase precision, personalize exposure estimations and source identification to enable prevention. A dynamic data infrastructure that can manage these (sensor) data flows in real time is required. In this research line a close cooperation with the IRAS institute of the UUtrecht is formed. A joined post-doc will increase cooperation between TNO and UU.

Analysis and interpretation of internal exposure data and integration with model: Presently, there is a lack of insight in how combinations of exposure patterns are related to personalized health effects at the individual level. Also, the effects of interventions (e.g. exposure reduction) cannot be directly monitored in relation to reduction of health risks or improvement of health. Internal exposure and effect data (e.g. biomarkers) and models can assist in bridging external exposure data towards health status.

Thus, the development of approaches is needed that enable: (1) the qualitative and quantitative linkage between external exposure to markers of internal exposure; (2) the qualitative and quantitative linkage between markers of internal exposure and biomarkers of health effects. The technological breakthroughs consist of: (1) the development of methodology and data infrastructures for identification of these biomarkers from literature; (2) the (co)-development of detecting these biomarkers towards ultimate application into (personalized, minimally-invasive) sensors.

Development of an environmental and occupational demonstrator: As the technology developments for sensor hardware and models for data interpretation know their own challenges and research questions, both are brought together in demonstrator systems. These are systems which for well-defined applications, bring together the sensor hardware and the data infrastructure. These demonstrators have the character of proof of concept setups. The first

[2] http://ec.europa.eu/environment/air/quality/standards.htm

demonstrator system will be one for occupational setting identifying different chemical compounds in PM. The second demonstrator will be one for the general environment air quality monitoring and again chemical composition of PM. The third demonstrator will be again for occupational setting, however compared to the first system this one will have been miniaturized to enable personal usage.

4. Applications and partnerships

Applications for the technologies and systems developed can be found in two main categories:

i) Occupational settings: warning employees and employers if limit values of hazardous substances are reached. This advice should be given on a personal level or at least on small group level to persons working together.
ii) General environment: giving personalized advise 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.

For both application areas PM has been chosen as first concrete example, since it related directly to respiratory complaints and is a large burden of disease (4% of all of NL).

<u>Occupational application:</u>

For the occupational application a joined study together with NIOSH and HSE has been carried out: 3 countries and 3 different settings. The data is available for all parties and is regarded as in-kind contribution of the two cooperating institutes.

Furthermore an interest group of 10 Dutch construction companies has been formed to guide the development of the TNO system. A field study is planned at Mateboer, one of the construction companies.

B2B projects have been realized with Casella (250KEUR realized and additional potential of 500KEUR). There is growing interest in the community and parties interested include Oxility and the Dutch defense organizations.

<u>General environment:</u>

For the general environment application TNO is partner in a measurement network in Eindhoven. TNO provides sensor systems, which will be installed at several locations. (100K/year for 3 years released OIT). The Eindhoven network can be used as testbed for new developments such as the ERP and future VP demonstrators.

Next to the B2B partners there are several EU-projects, which are related to the ERP: HBM4EU, EU Exposogas and since 2020 EPHOR.

On the modeling 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)

Plan Year 2021

A. Plan – Research Line "Sensor development for PM and VOC exposures"

A.1 Key results so far

A chemical identification method based on IR spectroscopy has been established. The technology is protected by 3 patent application (2019- 2020).First lab-demonstrations have been shown. As calibration facilities TNO labs in Petten and Rijswijk were used. Furthermore the principle of chemical identification in conjunction with cyclone and hollow waveguide technology to concentrate PM and align the particle and light paths for better measurability has been implemented in a first portable demonstrator.

A.2 Key objectives and expected results

In 2021 TNO's unique portable technology for chemical identification has to be miniaturized by a factor of 5 in order become wearable. For the miniaturization, new concepts of detection will have to be explored like plasmonic filters or MEMS FTIR. Concepts for the miniaturization will be worked out taking into account target costs of <2KEUR. The some of the research questions include: which materials will have to be used for the filters, can one work with broadband or small band radiators, and how to measure PM chemistry in other than crystalline silica?

Furthermore for the general environment sensor a new set of chemical compounds with their respective spectral peaks will have to be identified. The detection technology has to be tuned to the new compounds, with respect to concentration and infrared detection spectra. The limits of detection must align with the environmental regulations: ~1-100 µ<u>g/m3 for PM and</u> 1-100 ppb for hazardous VOC's

B. Plan – Research Line "Analysis and interpretation of external sensor data and integration with models (external exposome)"

B.1 Key results so far

For occupational exposures possibilities to develop sensor based dispersion models using CFD modelling or statistical interpolation techniques (Kriging) have been explored. Ultimately, these new dispersion models can be implemented in EXCITE(**EX**posome **C**omplete **IT**-**E**cosystem) as a method of automated analysis of sensor data to translate sensor data in near real time into (predicted) concentration maps of a workplace and presents this feedback to e.g. workers through app or dashboard. We are not yet there though. In parallel, the use of so called context sensors is explored. Once synchronized with exposure sensor data, these context sensor data assist in the interpretation of the exposure data with respect to when where an why exposure occurs. EXITE facilitates the analysis of exposure and context data and once known how to use the context data the interpretation can be automated.

EXCITE is being developed. This data infrastructure can collect and store sensor data of connected sensors, synchronize data from different devices, enables data analysis to translate data into information on one hand, but also facilitates automated analysis in near real time once the algorithms are known and provides the possibility to give data based feedback in near real time through an app or dashboard. Excite offers the possibility to combine sensor data with models.

With respect to environmental exposures, the resolution in time and place of the models is increased. A connection between LOTOS Euros and Urban Strategy has been realized. Herewith, an increased resolution of background concentrations is achieved, but also the possibility to identify sources contributing to the concentration at specific time and place is created. An evaluation of this advanced method for air quality assessment is performed, both for the city of Amsterdam as well as for individuals. Methods to improve model based estimations with available measurement data (either station data or sensor data) have been explored. Ultimately these methods can be implemented in EXCITE to provide advance personal exposure estimations as well as prediction. Last but not least, because quality of model outputs depend on quality of model inputs, new methods to estimate and predict emission from traffic with high resolution in time and place have been implemented, covering a much larger region (NL complete, compared to city regions before).

B.2 Key objectives and expected results

In 2021 a study focused on (personal) environmental exposure will be performed in Eindhoven. Eindhoven is growing and re-developing and maintaining during which enhancing a healthy living environment for its citizens is an important criterium. In this context, the ERP intends to demonstrate the use of its technological and methodological developments on one hand to predict the health impact on the population of Eindhoven of the intended urban development plans (combination of Urban strategy with information on population dynamics and demographics) and on the other hand to make visible to individuals what their personal exposures are and how their own behavior can contribute to reduce these exposures (by source apportioning). Key objectives for the ERP are:

- Based on GPS tracks of individuals their personal exposure to PM (and possibly other air pollutants like BC, NOx, VOC) will be estimated and predicted +3h with the advanced models of Urban Strategy (including source apportioning).
- Using available measurement data (LML network, ILM 2.0 network, mobile (sensor) networks) methods will be developed and implemented in EXCITE to upgrade the model estimations and predictions into more accurate values.
- Validation of the model estimations will be done against measured values (both stationary and at individual level).
- Feedback (actual exposure, prediction for +3h and advice) will be given to the individuals via an app, using EXCITE.

Even though the key objectives for the ERP are clear, further refinement is required to specify the exact focus and content of the demonstrators. This especially holds true for the chemical identification of PM exposure. In collaboration with the municipality of Eindhoven and the province of N-Brabant, but also with the citizen initiative Aireas we need to identify substances of interest in environmental dust (PM) sources like traffic (BC, PAH) and agricultural dust (pesticides, endotoxins, crystalline silica). We intend to present our plan to the Eindhoven consortium in October 2020, providing an opportunity to discuss the substances in PM that ask special attention. In preparation of a second demonstrator for occupational application in 2022, the work on dispersion modelling (CFD and Kriging) as well as on context sensors will be continued in 2021.

C. Plan – Research Line "Analysis and interpretation of internal exposure data and integration with models"

C.1 Key results so far

The aim of the ERP is to find biomarkers of exposure and/or of disease that can be measured non-invasively. Currently identified biomarkers for PM exposure or PM related disease are 1) not very specific and 2) only measurable in blood. Therefore we developed and applied a new text mining and AI approach (BDC/INDRA) to find additional biomarkers. This resulted in a list of candidate internal biomarkers as indicators for exposure to (specific types of) PM or diseases related to (specific types of) PW. The next step is to validate these newly identified biomarkers. Because one of the preconditions is non-invasive measurement, the biological matrices in which the candidate markers are present were identified. Moreover, an inventory was made of companies that develop sensors that measure non-invasively. These two criteria were used to select candidate markers for validation.

A cohort study carried out by the University of Aarhus (DK) is containing the measurements needed to experimentally verify some of the identified biomarkers. IP and contract negotiations with Aarhus are ongoing and planned to be finished before the end of 2020. Other initiatives (e.g. EPHOR, validation on existing data) are being explored.

C.2 Key objectives and expected results

In 2021 experimental verification of the selected candidate biomarkers will take place, either through the Aarhus cooperation or within the EU project EPHOR. Depending on the evaluation results and the biological matrices relevant for the evaluated biomarkers, companies will be selected and contacted for collaboration in a new project outside this ERP that aims to develop a non-invasive sensor for these biomarkers. This trajectory should take place in 2021 – 2022.

D. Plan – Research line “System integration: Development of an environmental and occupational demonstrator”

D.1 Key results so far

A first demonstrator (stand-alone version) for chemical identification of crystalline versus amorphous silica has been built and subjected to a field test. Chemical identification was successful and integration of the results in the data infrastructure is ongoing. Another field test at a construction company (Mateboer) is planned for wk 42 2020, where the connected sensor devices and data infrastructure will be tested.

D.2 Key objectives and expected results

A second demonstrator for general environment will be build. Challenges are the multitude of chemical compounds in PM (not only crystalline silica) and the combination with software for source identification. Furthermore data from other sources (like city networks will integrated in the data infrastructure giving the TNO demonstrator unique capabilities. The demonstrator will be tested at TNO and integrated at one test site of the Eindhoven network. In addition, the data infrastructure will be used to combine models and measured data and provide feedback to individuals or the community

FRONTIERS-Optical Satellite Communication

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Program description

1. Problem definition

Our Digital Society will require an omnipresent, ultra-high broadband communication infrastructure, which fully supports its information-oriented characteristics such as Cloud Computing, the Internet of Things, the Internet of Everything and High-speed Connectivity. To illustrate this, the European Commission has formulated her vision and policy actions to turn Europe into a **Gigabit Society**, as a follow-up of the Digital Single Market and the Digital Agenda for Europe. The main objectives of the EU Gigabit Society are:

- Gigabit connectivity for all main of socio-economic drivers,
- uninterrupted 5G (and beyond) coverage for all urban areas and major terrestrial transport paths, and
- access to connectivity offering at least 100 Mega-bits-per-second for all European households.

For the Digital Society, the data communication needs are growing exponentially. With respect to Internet traffic for instance, Cisco has predicted that the Annual global IP traffic will grow by 26% and arrive at nearly **5 Zettabyte** (ZB) in 2022. Other critical requirements for features such as availability, reliability, security, dependability and low cost are evolving in a similar fashion.

With respect to **security** specifically, the EU has launched the Quantum Communication Infrastructure (QCI). A pan-European QCI system aims at covering, from a public sector perspective, the domains of: (1) Inter and intra EU government communications, (2) Data centres interconnections and (3) the Critical infrastructure. On national level, free-space optical communication is an important technology in the **KIA Veiligheid** (MMIP 3.4).

Satellites and also aerial and maritime platforms will play a crucial role in the overall communication network. Complementary to the terrestrial network, a satellite network offers key capabilities such as: instant, flexible and global coverage and secure links over long distances. The field of Satellite Communication finds itself at the brink of a technological revolution: the transition from Radio-Frequency (RF) waves to Optical waves.

The **disruptive step** from RF to Optical Satellite Communication will enable various strong advantages, such as much higher bandwidth, very high data rates, quantum key distribution and immunity to interception.

2. Positioning

In the past 5 years, a worldwide increase in technology development for optical satellite communication is taking place as the communication market is becoming ready for the disruptive step towards optical wavelengths. TNO is working towards a prominent position in this field, on the basis of the very strong and long-standing (> 50 years) track record in optics, mechanics and mechatronics for Space and Astronomy instrumentation. Currently, TNO is realizing first generation prototypes for various ground-, air- and space communication terminals, together with a (Dutch) supply chain and in collaboration with large system integrators such as AirbusDS, Tesat and Thales. Parties competing to TNO in this field are DLR, Fraunhofer, Onera, SME's such as Mynaric and Synopta and applied research at MIT in the US.

The ERP aims to build the knowledge and technology fundaments for (long-distance) Optical Wireless Communication. The ERP targets the design of both **innovative system concepts** and **key building blocks** with a performance which is *unmatched* worldwide. The design requirements are set 'an order of magnitude' better than what is currently being developed. This will lead to significantly improved prototypes and products in 5-10 years from now.

The ERP can involve the broad range of relevant expertise present at TNO (mainly from Industry, ICT and DSS) into the program and moreover – based on the well-established system architecting capabilities – create innovative system concepts for various communication links. Primary TNO knowledge fields include: Optics, Photonics, Mechanics, Mechatronics, Atmospheric Physics, Quantum technology, Network and communication technology. The focus of the research is on technology for the physical layer (ref. OSI model) and to a lesser extent on the data and network layer.

The close connections to a wide range of Dutch and international industry partners and with ESA enables the ERP to carefully select and validate the research directions and targeted concept products. On the fundamental research side, a large program on this topic is being submitted to NWO Perspectief (Sept 2020). The ERP envisions to collaborate with ~5 university groups in this fundamental research program.

3. Objectives and approach

The main objective of this ERP is to build a very strong knowledge and technology position in Optical Wireless Communication, with emphasis on Fast (high data throughput) and Secure (quantum encrypted) communication. Furthermore, the ERP aims to:

- Design novel and strongly improved concepts of systems (ref. state-of-the art)
- Focus on key technology building blocks
- Co-operate with university groups for high risk / high impact developments
- Optimize and combine technology developments to selected communication cases
- Seek other applications and cross-overs
- Demonstrate tech development in the lab, on (sub-) system level – reaching TRL4 by 2023.
- Follow up by a continued development with Dutch and International industry and to contribute to the very strong business case of Dutch industry (see Section 4).

The ERP has a focus on the following research fields:

a) Low loss Free-space optical channels, enabling ultra-high data throughput and high key rates
b) Mitigation of intensity fluctuations (scintillation) and fading
c) Data modulation and multiplexing for high data throughput
d) Modeling of atmospheric turbulence behaviour – the statistical behaviour over long periods
e) Beam tracking and steering pointing under highly dynamic conditions
f) Technologies for multi-point communication
g) Orchestration of network traffic
h) Large Field-of-View, large aperture, low wavefront error telescopes and optics
i) Free-space quantum channels, enabling high secure key rates
j) Optimization of Signal-to-Noise in photon-starved conditions/in day-time operation

The output is to be formalized in various IP-formats: patents, copyrights and know-how depots. This should lead to fee and royalty incomes on the longer term.

A research collaboration of TNO, with academic partners, institutions such as ESA, and industry partners is pursued, focused on the development of knowledge and technology for future optical wireless communication products. On the fundamental research side, co-operations with university groups are being built up to address the more fundamental, high-risk/ high impact research challenges. The university partners are:

- TUDelft: Opto-Mechatronics, Optics, Space Systems
- TU Eindhoven: Electro-Optical Communications, Control System Technology
- UTwente: Communication Systems, Pervasive Systems, Photonics Systems
- UnivLeiden: Astronomy Instrumentation
- VU A'dam: Theoretical Physics

Within the program proposal "Optical Wireless Superhighways" towards NWO Perspectief, 5-6 PhD projects with these universities are planned.

On the application side a close interaction with industry is taking place. ERP technology concepts are to be matured further in a continued development with Dutch and International users and industry. In follow-up phases, partial funding should come from industry and the other part for this phase could be provided by SMO, TKi, EU or ESA. After that, the product realization phase starts which is led by industry, and in which TNO could have an advisory role. Industrial development partners can be large system integrators, satellite operators and service providers, or are suppliers of optics, photonics, mechatronics, electronic or space equipment.

The ERP research lines of High-data throughput and Ultra-secure communication have a strong connection to the topics and technologies in the following TNO roadmaps: Unit Industry – Roadmap Space and Scientific Instrumentation; Unit DSS – Roadmap Information & Sensor Systems, Roadmap Protection, Munitions & Weapons; Unit ICT – Cluster Fast Open Infrastructures, Trusted ICT.

4. Applications and partnerships

The driving application field is Optical Wireless Communication over long distances. This comprises the specific communication links:

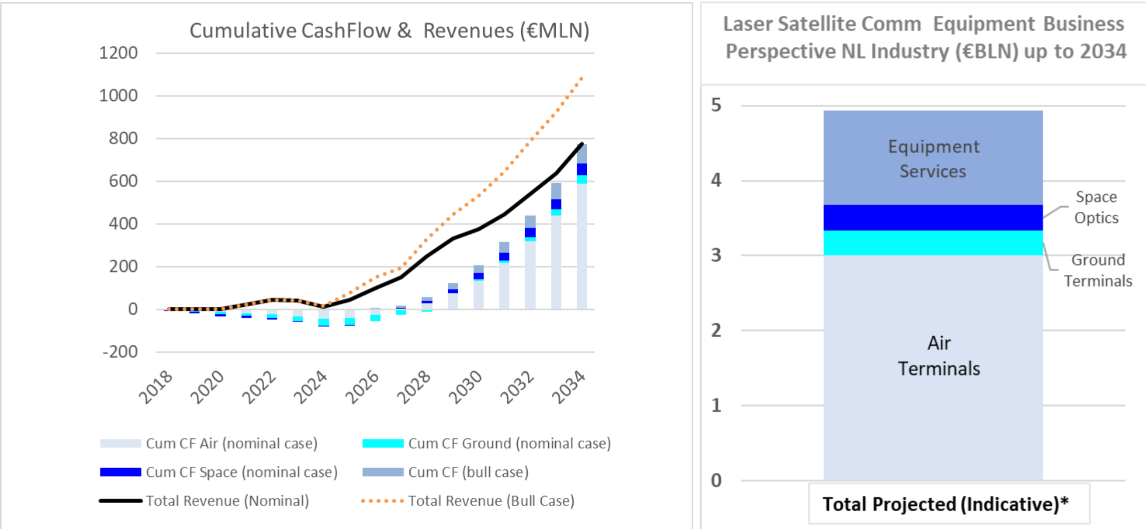
a) Ground-to-satellite (Low Earth and GEO-stationary orbits) links
b) Inter-satellite links
c) Links to air- and maritime platforms

d) Quantum Key Distribution links
e) Terrestrial wireless links

Partners

A. University: TUDelft, TU Eindhoven, UnivTwente, VU Adam, Univ Leiden.
B. Institutional: ESA, NASA, DLR, NCT
C. Industrial, per category:
   - Large System Integrators: Airbus, Tesat, Thales, OHB
   - Technology suppliers: Demcon, Nedinsco, Hyperion, VDL, Hittech, Lionix, Aircision, Celestia, ..
   - Communication Service providers: Eutelsat, Viasat, SES, Immarsat
   - Telecom providers: KPN,
   - Users: financial (ABN), MODs, Governments, …

The impact of the ERP technology innovation is best illustrated by the expected, long-term revenues and cash flows for Dutch industry in this field.



Optical Satellite Communication Equipment Business Perspective for NL Industry. Left: cumulative cash flows and yearly revenues. Right: cumulative revenues up to 2034. [Source: Niel Truyens, Business Development Space]

The main impact of the ERP is to help Dutch industry realize the foreseen revenues and profits in Optical Satellite (and Air) Communication. This is a long-term effect which holds even beyond 2034.

A short-term impact of the ERP for users and industry is:

- Concept designs for future communication terminals, at ground, in air or in space.
- Profound insight into critical technologies for future communication links and their development roadmaps.
- Novel and state-of-the-art (Top of Europe/ World) key technologies to strengthen market position.
- Laboratory verified technologies for further co-development by TNO and industrial partners.

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The research activities for Ultra-high data throughput and Ultra-secure communication are shown in the Table below. Also the quantitative performance targets are indicated. The references are represented by world-wide state-of-the-art systems.

A. Ultra High Data Throughput		
- Terabit per second links	Key Results so far	improvement wíth respect to reference
	System concept for a 10 Terabit/s Ground to GEO satellite feeder link	10 times higher data rate
	High power beam combiner system; up to 50 beams of 50W each	50 times higher power enabled for 50 channels
	High-order data modulation and coding approach	10 times more data in 20 nm Erbium window
	Strategy for mitigation of irradiance fluctuations in open-loop setting	5dB reduction in link loss
	Network orchestration for traffic switching and splitting over multiple ground stations	10 ms recovery time
	Key Objectives 2021	
	System concept for a ~Terabit/s Ground to LEO satellite feeder link	30 times higher data rate
	Turbulence statistics model and computation tool	accurate estimate of Cn2 moments
	Adaptive transmission strategies based on Channel State Information	5 dB reduction in link loss
	5G network for LEO constellations	novel protocol
- Multi-point Communication	Key Results so far	
	Two System concepts for multi-beam communication terminal at a GEO-satellite	reduction of SWaP by factor 3 (@10 links)
	Large Field-of-View, low aberration transmitter and receiver telescope design	8 x 3.2 degrees FoV with low wavefront error
	Dynamic tracking system for aircraft links	up to 100 parallel targets
	Key Objectives 2021	
	Detailed design of satellite multi-beam receiver and beam steering system	TBD
	Experimental verification	
B. Ultra Secure Communication		
	Key Results so far	improvement wíth respect to reference
	QKD protocols performance analyses, in the presence of channel loss and noise	not applicable
	Concept design LEO QKD service	optimized contact time
	System concept for background noise filter for high key rate and day-time operation	3dB improved Signal-to-Noise
	Technology Concept for laser phase locking to handle large channel loss	allows for 25 dB higher channel loss
	Key Objectives 2021	
	Detailed design for extreme background noise filter	3dB improved Signal-to-Noise
	Experimental verification for extreme background noise filter	
	Detailed design for phase lock system	allows for 25 dB higher channel loss

Wise Policy Making

ERP Contacts: J. Sassen (Project Lead), H.-J. van Veen (Science Director)

Program description

1. Problem definition

In the midst of a pandemic and heading towards the largest economic recession since the 1930's, the demands on policy-makers and government officials are extremely high. Many of the policy options in a crisis are 'wicked' in nature: The complexity of issues is overwhelming, the potential side effects unclear, and the arena's in which the policy discussions take place are ambiguous and volatile. The current Covid-19 crisis demonstrates this reality painfully. And it is not likely an isolated incident, but more probably indicative of what lies ahead for policymakers. The Netherlands is at the dawn of several other major, radical changes driven by e.g. climate change (the energy transition), technology (autonomous driving, Artificial Intelligence, surveillance, cryptocurrencies), national developments (population aging), and globalization (migration, new pandemics).

In order to get a grip on these overwhelming developments, policymakers and citizens alike are faced with some fundamental questions: How can we - endowed with all the currently available science, data and technology - aim at improving (or re-gaining) our nation's level of wellbeing? What policy options will guarantee a future in which its people and other living beings can flourish? How can we know - and agree upon - what this future looks like? And how do we choose policy options that steer towards this future?

Policymaking that accounts for the wellbeing of our society, now and in the future, is essential to effectively manage the radical changes of the current crisis, and the crises to come. Steering towards wellbeing is in line with an important forthcoming and global (though mostly Western) trend in policy making best known as 'beyond GDP': the acknowledgement that GDP captures a relatively narrow aspect of wellbeing, i.e. economic growth — and that we need a new set of indicators that capture a broader range of sustainable wellbeing.

There are, however, currently only few and partial instruments available to assess the expected impact on wellbeing prospectively. Policymakers generally use frameworks like social cost-benefit analyses when weighing up the various policy options. However, many limitations are still encountered when trying to properly assess wellbeing, which is why it is often not fully considered in analyses. Unlike amounts of money, wellbeing is considered more difficult to translate into data that can be easily compared. This is complicated even further when trying to compare conflicting forms of wellbeing (like 'privacy' versus 'safety'). Another hurdle that is recognized in policymaking, is that the policy making process is characterized by insufficient attention and guidance towards unbiased dialogue and towards creating consensus among multiple stakeholders, citizens, and other involved participants. With a lack of solid and reliable data on the effects of policy options on wellbeing, adverse effects of cognitive biases and vested interests in policy discussions are imminent.

This ERP aims to fill this gap. Our aim is to develop a suite of instruments and methods to support policy makers to assess the impacts 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 believe that policy-makers who are steering towards prioritizing wellbeing deserve the very best support. It is thus time for the Netherlands, to join the front-runners and be one of the first countries in the world to raise its standard of policy-making. By using hard data from scientific models, and then using well-supported 'wise deliberation' to examine the value of this data.

2. Positioning

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'.

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.

3. Objectives and approach

Our ambition for 2022 is to deliver a prototype (TRL 5) of a ‘Wise Policy Suite’ of instruments and methods that is tested and validated in practice, and is geared towards practical use by policy makers. With this Wise Policy Suite, we will be able to assist policy makers 1) 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. This will enable them to develop and choose policy options that maximally promote wellbeing, based on scientific insights ánd legitimized by society. There are 3 main lines of research:

WISE Cube: Providing a reliable tool that helps to assess the impact of policy options on wellbeing by quantifying the impacts on wellbeing. Based on the work in 2019-2020, we will further develop our current prototype from TRL 3 to TRL 5 to assess the impact of policies on choice of options and the impact on wellbeing using valid wellbeing models and data. 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 outcomes of the WISE Cube offer prognoses of the expected impact on wellbeing for various policy scenarios explicated for the different target groups.

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 based on outcomes of the Cube. 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 values and knowledge that are relevant for the policy options. The arguments for and against options, and the underlying facts, knowledge and values, are registered so the decision of the W.I.S.E. Tank is transparent, explainable and can be stored for later reference. In this way, the W.I.S.E Tank complements the outcomes of the W.I.S.E. CUBE by supporting policy discussions on the outcome of the WISE Cube.

Policy Practice: Tuning the above developments to concrete use in the actual policy practice. This line of research encompasses an extensive case study on how wellbeing 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 (demonstration, evaluation). 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 advantageous to see if we can also address a case study in that field.

4. Applications and partnerships

Partnerships:

This ERP intends to build partnerships with the Dutch ‘Planbureaus’ and the WRR. We are currently discussing the possibilities for a collaboration with representatives of the following bureaus: PBL (Planbureau voor Leefomgeving), SCP (Sociaal Cultureel Planbureau), CPB (Centraal Planbureau), and the WRR (Wetenschappelijke Raad voor Regeringsbeleid). These bureaus have a very good rapport with government officials and policymakers and they are involved in advising government, DOC and the ‘Tweede Kamer’ as well as preparing large government plans such as the ‘Miljoenennota’ and ‘Prinsjesdag’. The CPB also collects large amounts of data, some of which are on wellbeing-related issues.

This ERP is working on a partnership with the following universities/professors:

- Emeritus professor Ruut Veenhoven & Dr Martijn Burger (Academic Director) of the Erasmus Happiness Economics Research Organization, Erasmus University of Rotterdam
- Dr. Mr. Niek Mouter, TU Delft, Appraisal Methods for Transport Policy and Planning
- Technical University of Vienna, Stefan Woltran, Institute o Logic and Cmpuation, topic of cooperation: Implementation of Argumentation Framework, Framework Visualization
- University of Helsinki, Andreas Niskanen, Department of Informatics, topic of cooperation: Explanations and Diagnoses in Formal Argumentation Representation.

Applications:

- Patricia Zorko (deputy NCTV) and HP Schreinemachers (Director of Analysis and Strategy) have expressed their enthusiasm about the potential of the ERP knowledge for the NCTV (Nationaal Coordinator Terrorismebestrijding en Veiligheid). We are currently conducting a short inventory together with the NCTVto see how the WISE Cube can be customized for their specific needs. The intention of the NCTV is to take up a line of research in which the WISE Cube can be made useful for ‘counter-terrorism’ and/or for ‘Crisisbeheersing’ in their VP (Vraaggestuurd Programma) of 2021. (Roadmap National Security, unit DSS). Also the potential of the Wise Tank may be explored.
- The municipalities of Rotterdam, Amsterdam and The Hague and the Ministry of Infrastructure and Water-management have expressed their interest in working with wellbeing parameters and the WISE Cube for Mobility related issues. (Roadmap Sustainable T&T, unit Traffic and Transport)
- TNO and the municipality of Rotterdam are now working on a SOK (Strategische Samenwerkings Overeenkomst) on accessibility, air quality, sustainability and energy transition. The knowledge on wellbeing measurement and evaluation that has been developed in the ERP will be applied in a Mobility project that is currently being developed within the SOK. (Roadmap Sustainable T&T, unit Traffic and Transport)
- Veiligheidsregio Rotterdam-Rijnmond and Brabant may be interested in the Wise Cube, while the attention has shifted to effect-based policymaking, long-term effects and impact on well-being due to the Corona Crisis.
- The Ministry of I&W is interested in setting up a case study to apply the WISE Cube in studying the introduction of new mobility concepts. (Roadmap Sustainable T&T, unit Traffic and Transport)

Plan Year 2021

A. Plan – Research Line “W.I.S.E. Cube”

A.1 Key results so far

- A web-based prototype (TRL 3) to support policy makers in assessing the consequences of policy options on human mode choice and wellbeing for groups in society that integrates 1) an enhanced version of Marvel (semi-qualitative modelling), 2) our enhanced Discrete Choice Model (quantitative modelling) with a unique database of transport mode choice in the Netherlands and 3) an algorithm to calculate elasticities.
- A conceptual demonstrator (TRL 2) of the Wise Cube Dashboard is developed to support awareness of policy options and effects on wellbeing of societal groups in an intuitive way.

A.2 Key objectives and expected results

A web-based prototype (TRL 5) that additionally includes 1) a library of wellbeing models for marvel modelling, 2) functionality to collect, analyze and visualize wellbeing data and 3) the Wise Cube dashboard that supports the awareness and evaluation of policy makers of the effects on wellbeing of policy options on societal groups in an intuitive way.

B. Plan – Research Line “W.I.S.E. Tank”

B.1 Key results so far

Dialogue support

- Inventory of the most useful methods for formal dialogue representation, its analysis, querying and visual representation as well as the available software for their implementation .
- Neuroevolutionary bias framework and wisdom framework which enables to develop advanced working- and dialog forms aiming at wise decision making on complex issues.

Fostering wisdom

- Insight into the most prominent factors determining (collective) wisdom in general, and more specifically, how evolved characteristics of human judgement and decision making (cognitive biases) hamper wise decision- and policymaking.
- Report and peer reviewed publications that show that cognitive biases are robust phenomena that may counter effective policy making with regard to sustainability treads.

B.2 Key objectives and expected results

Dialogue support

- Proof of principle for the representation, consistency analysis of the represented knowledge and values, as well as querying the representation on argumentation supporting or attacking a knowledge or value statement
- Specification and evaluation (evidence-based) of dialogue forms (or formats) and other kinds of interventions that support people to engage in debiased dialogues, about complex problems taking into account values, (lack of) knowledge, and facts. Handbook with dialog forms.

Fostering wisdom

Development of tools and influence techniques to promote wise, sustainable choices and behavior in the context of the current, modern world. This will focus on an approach using environmental interventions (deliberation forms, formats, nudges, and influence techniques) promoting the necessary preconditions for fostering collective wellbeing.

C. Plan – Research Line "Policy Practice"

C.1 Key results so far

Governance level: Scotland case study

Knowledge on the establishment and functioning of the National Performance Framework (NPF) of Scotland – a comprehensive, all levels of government-encompassing tool for implementing and monitoring wellbeing as a broader national goal. Insights into the challenges and opportunities policy makers, institutions and stakeholders face when setting-up nation-wide wellbeing policy agendas and regulation mechanisms. Identifying knowledge frameworks, models and tools used in the translation of abstract wellbeing objectives into implementable practices on local level and learning from best practices of community engagement and consultation.

Domain level: Mobility case study

An overview of policy practice on wellbeing in the domain of Future Sustainable Mobility and the use of assessment mechanisms, decision making models and indicators.

C.2 Key objectives and expected results

Governance level: New Zealand case study

Having drawn useful insights from the case of Scotland, we intend to conduct another in-depth study into New Zealand's wellbeing policy-making and respective budgeting. By tracing New Zealand's efforts in defining and measuring the nation's wellbeing we aim to complement our knowledge on working implementable models from the practice.

Domain level: Mobility case study

Understanding current policy opportunities on the implementation of wellbeing in ex ante evaluations. Setting up case studies with municipalities and ministry I&W to experiment with WISE Cube applications in an iterative cycle of innovation.

Sustainability And Reliability for PV & (opto-)electric thin-film devices

ERP Contacts: A. Kuypers (Project Lead), M. Theelen (Lead Scientist), A. Faaij (Science Director)

Program description

1. Problem definition

The societal impact of optoelectronic devices is enormous, and will continue to grow rapidly. In the form of devices for photovoltaic energy generation, sensors, data transport, and computing, as well as in lighting and displays, optoelectronic materials play an ever more critical role. Therefore the reliability of these materials, which are typically tailored on a micro- and nanometer scale to enable their desired functionality, is crucial. Moreover, because of their abundant application all such devices tend to evolve from high added value systems to commodities which are embedded in the lasting infrastructures we rely on.

Focus will be on solar cells as a prominent example. By 2050, about half of the worlds electricity production may depend on optoelectronic PV materials, with critical dimensions well below the micrometer range while requiring a product lifetime of 35 years or more. In principle, such lifetimes are required for all types of solar cells (crystalline wafer-based as well as thin film), because the desired future scenario is to combine these technologies in tandem configurations with superior efficiencies. To maintain public acceptance when installing vast areas of PV, the national roadmap (IKIA, MMIP2) is focused on integration of PV in multifunctional surface areas of buildings and infrastructure or floating on water, implying multiple stress exposure of devices. The vast scale of PV deployment (up to km^2) provides a unique opportunity to achieve the project objectives, as degradation on nanometer scale can be studied with statistics on km^2 scale.

2. Positioning

Generally speaking, the existing state of the art in reliability of (opto-)electronic thin film devices has been developed for high added value domains: specific handling, installation and use, as well as environmental conditions are prescribed to protect the device and to optimize its performance and lifetime. In the case of PV, this means that current state of the art is based on standardized, one-size-fits-all crystalline silicon based PV modules, which are used in dedicated environments (in solar fields or mounted on roofs) where external stress factors are limited to light, heat, humidity and hail. Quality control based on these stress factors has been developed to a level that lifetime guarantees of 15-25 years provide sufficient credibility for investors. A detailed phenomenological catalogue of lifetime predicting properties and failures exists, in some cases also with a model-based understanding of underlying mechanisms. State of the art for devices like sensors, displays and lighting is comparable. However, for thin film devices the state of the art in reliability lags behind, and much less basic understanding exists. Both in crystalline and thin film PV, as well as in thin film flexible sensors (stretchable interconnects) reliability research at TNO is world class. We have beyond state of the art facilities for accelerated multiple stress testing, world class field testing facilities for (integrated) PV and long term collaborations with equipment companies, PV producers, as well as service companies providing reliability testing and due diligence (including the main gate keepers of the Dutch solar market).

Now that such opto-electronic devices are becoming cheap commodities, they are increasingly used in (integrated) applications where they are exposed to multiple stress factors. These are rapidly expanding markets, where little is known about degradation mechanisms induced by additional stress factors and innovative PV devices (bifacial Si, tandems, Perovskite, integrated PV). The trend for (wearable) integrated sensor systems is similar. Accelerated life time testing should be performed in the lab, under representative multiple stress conditions. To accelerate the development of a phenomenological catalogue of failure mechanisms, and to detect underlying degradation mechanisms, we employ a novel and unique approach, referred to as “coring”. Together with PV developers, installers, owners, and field inspection service companies, we detect malfunctioning modules in the field. By coring, we isolate affected cell elements while keeping them intact, and those functional cells are studied in the lab to identify defects and their possible cause. Following such “post mortem analysis” we perform multiple stress accelerated lifetime tests, to clarify the underlying degradation mechanisms. On main issues, we extend research by PhD and postdoc positions, thereby also extending our university partnerships.

By coring, we thus create a unique bridge between large area field statistics and nanoscale lab analysis. Moreover, the sample preparation by coring involves the removal of the encapsulation materials of the device. This disassembly step generates insight in potential recycling processes, and (especially relevant for integrated devices) enables us to experiment with materials/designs optimized for disassembly. This combination of lifetime performance and recyclability will be studied to formulate a TNO position and strategy on the development of integrated opto-electronic (PV) devices in the novel EU framework for Ecolabeling.

This ERP thus serves TNO to advance its position in 3-4 Roadmaps:

- Solar Energy: Understanding of degradation mechanisms under multiple stress; Improved PV design/reliability/predictable lifetime; proprietary methods for analysis (coring) and disassembly
- Flexible freeform products: Improved design and lifetime of flexible thin-film devices and stretchable interconnects
- Sustainable society: Position paper and research approach on ecodesign and recyclability (especially in built environment)

3. Objectives and approach

To improve reliability, 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 will be used to guide accelerated lifetime testing in the lab, in combined-stress tests.

More specific objectives of this ERP in 2020 are to develop a more basic understanding of relevant degradation mechanisms at (1) the interfaces of and within the active and functional layer materials (CIGS, PSC, cSi, sensor materials), 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. This basic understanding will facilitate smarter choices of encapsulation (cost effective / fit to purpose / flexible / designed for disassembly) and integration. A TNO position paper will be written concerning sustainability and circularity of integrated PV and other optoelectronic devices, connecting to the European actions on Ecolabeling.

Research line 1: Reliability

The qualification and attractiveness of a solar panel or optoelectronic device is primarily determined by its performance, costs and lifetime. Any product will be exposed in its operational lifetime to external stresses like humidity, temperature, mechanical deformations, chemicals, electric currents, radiation, hail storms, wind forces etc. which will lead to a gradual decrease of the performance and in some cases to (unexpected) catastrophic failures. It is evident that it is desirable to minimize the degradation as much as possible and even more important, to be able to predict degradation phenomena so that measures can be taken before the product fails. It will also enable a more accurate description of the expected service life of the product.

Hence, in this ERP the long term goal is to be able to predict and prevent the occurrence of small and large failures in (integrated) optoelectronic devices. This will enable a decrease of the degradation rate and an increase of the lifetime. This will be reached by:

- A more **fundamental physical and chemical understanding** of failure mechanisms by performing post-mortem analysis for selected cases. This will lead to understanding how failures initiate and propagate in material stacks. Special attention will be on vulnerable spots such as interfaces where components are joined and different materials are combined. Both quantitative and qualitative schemes describing the mechanisms will be presented. The knowledge will be used by colleagues and customers to develop **novel materials- and process solutions to improve reliability and durability**, thereby strengthening TNO's technology proposition in PV and flexible electronics (i.e. product, enabler, service) and increasing market impact in specific domains of device integration.
- The development of **accelerated test protocols** for new types of flexible or rigid 3D-shaped devices in emerging application areas (like BIPV, Infrastructure Integrated PV, PV on water, Mobile PV, flexible sensor arrays and devices with stretchable interconnects) based on the fundamental understanding of material and interface degradation with results that can be translated into real life performance predictions. Special attention will be given to post-mortem analysis of devices that have failed under actual field conditions.
- A further strengthening of our image as an internationally recognized institute in this field of research and our position as partner in new joined commercial and scientific projects by playing a prominent role in international task forces and platforms like PVQAT, IEA PV task 13, ETIP-PV, PV-EERA for PV, and Photonics21, OE-A and EMIRI for flexible electronics.

Research line 2: Sustainability

The large scale introduction of photovoltaics and other optoelectronic devices should have a minimal environmental impact. This is important in the production process (carbon footprint, scarce materials), during the functional product lifetime, but certainly also after decommissioning. The large scale recycling of PV modules will therefore become important within the coming decades. The potential market size for PV module recycling is estimated to be 15 billion dollars in 2050. As large scale PV production just started in he last decade, and product life time is typically 2-3 decades, PV recycling has not yet developed to an economic scale. However, recyclability and separation of waste streams is already an issue, especially when the PV is integrated into products, construction components and buildings.

Goal of this (rather exploratory) ERP research line is to position TNO in this field and to identify strategic opportunities where TNO could make an impact. In order to address circular economy aspects and reduce the environmental footprint of (integrated) PV and other optoelectronic devices, in 2019 the first contours of a long term TNO strategy for sustainability have therefore been drawn by identifying the key drivers, opportunities and market chances with the aim to initiate a separate R&D program for this theme. The direction chosen is to connect to the European actions on Ecolabeling, and to explore promising routes for design for disassembly of integrated devices. In the current year 2020, a TNO position paper will be issued on the basis of a literature study in which market and technology development, as well as Dutch and EU policy and regulatory framework are assessed. We will present this position paper not only by using international platforms like IEA PV Task 12 (where TNO is already actively participating), and in national PV consortia and media, but we are also contemplating to condense it to a short video.

TNO scientists (representing teams in 5 departments from 4 TNO units):

- TNO Lead scientist Mirjam Theelen (ET-STA Solliance): international top position in understanding (multi-stress) degradation of (CIGS) thin film PV
- Senior scientists Piet Bouten (IND Holst Centre; reliability stretchable interconnects care and medical) and Jan Kroon (ET-SE Petten; reliability PV)
- TNO consultants Mara Hauck (Utrecht; Sustainability and circular economy), Sanne van Leeuwen (BIM Delft)

4 PhD’s, 1 postdoc, 1 research engineer (+ 2 PhD in process)

- TUD TNO-prof. A. Weeber + PhD Klaas Bakker (PV degradation and shadow tolerance)
- TUE prof. J. Hensen (BIPV) + PhD A. Bognar (CIGS BIPV outdoor performance and local shading)
- UT prof. J. Schmitz (semiconductor reliability) + Postdoc Pelin Yilmaz (Post Mortem PV analysis)
- RU prof M. Huijbregts + PhD M.v.d. Hulst (life cycle analysis)
- HELMo-CRIG Liège, promoteur P. Gabriel + research engineer J. Mahaux (life cycle assessment, eco-design and recyclability PV in roads)

Granted:

- TU/e Solliance A. Creatore PhD perovskite stability (NWO NEON):. Related Eindhoven Engine collaboration proposal “NEON Delivers” *not granted (communicated July 2020)*
- Interreg Sunovate: opportunity for UHasselt PhD Thermomechanical degradation (*vacancy*)

Not granted: ERC “IMMORTAL” (communicated April 2020; alternative funding is explored)

- *RU prof. J. Schermer + PhD Post mortem analysis*
- *UT prof. J. Schmitz + PhD Simulation degradation mechanisms*
- *TUE Assistant prof. Shuxia Tao + PD Modeling degradation impact on performance*

Expected before end of 2020:

- PhD on reverse bias in PSC (also for tandems), with TUD

4. Applications and partnerships

The TNO teams involved in this project are those of Solliance (STA), Holst Centre, MAS, SolarEnergy Petten (SE), and TNO Circular Economy (CAS). Participating universities are TUD (1 PhD active on partial shadowing), RU (1 PhD active on circularity), UT (1 Postdoc active on post mortem analysis), TUE (1 PhD active on CIGS field performance, 1 PhD starting on PSC stability), Nantes (F) (CIGS degradation) and HELMO (B) (1 researcher active on circularity for IIPV). The project combines the knowledge on PV with available strengths of TNO in the specific areas of integration (Building-, Road and infrastructure-, Agriculture-, Maritime-related demands) and TNO Circular Economy for the Sustainability topic. This provides a unique position for TNO to generate more insight in required specifications for PV lifetime and performance testing conditions, and to develop smarter integration strategies. Moreover, company partners of these groups are involved. A selection of national and international involved company partners are/will be Hanergy, AVANCIS (improved module design), Solar Tester, Eternal Sun, (tools for reliability testing) EigenEnergie.net, Soltech, Solinso, Exasun, ZigZag Solar (improved BIPV module design), DSM (encapsulation foils), Sabic, Tempress, Solmates, Levitech (improved PV process equipment), Dupont, Philips, Solvay, BASF and Henkel, as well as companies in the field of flexible sensors and electronics for medical and health care (partners in Holst Centre).

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The two research lines Reliability and Sustainability have become more intertwined as the project progressed, also because both the EU Climate Agreement and the now more specific Dutch goals for the Energy transition are putting increasing emphasis on the sustainability aspects associated with massive out roll of durable energy sources like photovoltaics.

General goal of 2021 will be to direct the methods and approaches so far developed towards more *sustainable* concepts to achieve predictable and improved reliability in *integrated* PV applications. An example of this is that novel encapsulants designed for more ease of disassembly (low temperature delamination at end of life) will be tested for reliability with respect to current state of the art. Industrial application of such encapsulants in BIPV is foreseen (parallel project with Dutch partners).

The sustainability agenda will be more specifically focused towards Building Integrated PV (BIPV). While working on the TNO position paper and the identification of strategic topics, we will also try to contribute more strongly to international task forces in this field (e.g. IEA Task 12, and the recently started EU Joint Mission Group Ecolabeling).

PV reliability work will be continued on thin film CIGS and wafer-based Silicon, by combining performance and degradation assessment in the field with ("postmortem") analysis/accelerated testing in the lab.

The unique approach of coring (diamond drilling) that now enables us to take functional test samples for lab analysis and testing, will be automated to some extent to make it more reproducible and less dependent on personal skills. To this purpose, some additional investments in tools will be made end 2020 (as part of the "Dream investments" made available by EZK). Apart from more reproducible sample preparation, this will also provide insight in disassembly for recycling.

In 2021, a second method will be added to further increase the impact of lab testing in detecting, identifying and understanding relevant combined-stress degradations occurring in the field. Starting in September 2020, the 2-year Interreg project "Sunovate" will start, with several work packages which are very well aligned with this ERP. Here we will perform continuous combined stress measurement by incorporating sensors inside PV modules which are exposed in controlled field labs (e.g. BIPV windows) as well as in PV test samples which are exposed to multiple stress accelerated lifetime tests in the lab. Specific goal of the project will be to demonstrate improved thermal control in glazing and solar modules for buildings, by modification of the module/glazing encapsulation material with thermochromic IR pigments. Both the effects of reduced IR heating and of the use of a modified encapsulant will be studied. We will collaborate with University of Hasselt (Prof M. Daenen) on the incorporation of FiberBragg sensors for temperature as well as mechanical stress detection.

Also, as part of the Dream investments, we will invest in internal relative humidity sensor systems, where intention is to collaborate with University of Ljubljana (Prof Topic).

A. Plan – Research Line Reliability

A.1 Key results so far

- Reproducible sample preparation by coring à unique knowhow on method (proprietary service)
- Reverse bias due to partial shadowing à tentative device designs to control ignition and damage
- Potential induced degradation in CIGS à diffusion mechanism mitigated by barrier layer
- Stability encapsulated PSC minimodule with TNO patented ALD à world record + publicity
- Understanding (modeling and validation) of localized deformation of printed conductive lines à Design rules for stretchable interconnects, applications in wearable vital sign patches and smart clothing + patent idea meander design
- >10 publications, >8 oral presentations
- Validation of several TNO patents with respect to reliability (e.g. ALD oxide layer for stabilization of PSC, Reduced side ingress of encapsulant due to ALD processing, Lamination foils with thermochromic nano-additives)

A.2 Key objectives and expected results

- Mechanisms reducing CIGS sensitivity to partial shading à design concepts
- PV testmodules with integrated sensors for combined stress monitoring (T, stress, humidity) installed at TNO field labs for BIPV, floating PV à unique approach to combine multi stress testing in field and lab.
- Lab and field testing of novel PV encapsulants with thermochromic IR pigments for thermal control, and study reliability effect on Perovskite modules (linked with ERP Submicron Composites in Interreg project Sunovate)
- Reliability performance of encapsulants designed for disassembly à durability of encapsulated contacts (T, RH, TC, PID) with respect to current state of the art; also bifacial, and novel TNO PLD-Metal oxides for silicon heterojunction cells
- Reliability and performance of stretchable printed conductors with integrated ridged components: Electrical performance studies during deformation including failure behavior of the interconnects à

design rules for stretchable interconnects to connect sensors on deformable inlays for PVs, stretchable health patches and smart textiles

Intended new partnerships and follow-ups

- TUD PhD “Reverse bias in perovskite”; builds further on first insights and methods obtained for PID in CIGS; this will be extremely relevant for Perovskite solar cells. Reliability research on reverse bias effects in Perovskite is totally unexplored, and TNO is uniquely positioned as we can make such modules in house. This work will be highly relevant to PSC and PV tandem ambitions in the core of the TNO Roadmap Solar
- Possibility to create a PhD position with Uhasselt (prof M. Daenen) “Integrated sensors for real time study of combined stress factors” within the framework of the Interreg project Sunovate.

B. Plan – Research Line Sustainability

B.1 Key results so far

- Literature study completed: mapping sustainability issues in PV domain with respect to Ecolabeling, Primary Energy Factor and the Energy Performance of Buildings Directive directives à public TNO position paper
- Update on state of the art in recycling of (integrated) PV à hardware investment choices for disassembly of samples and modules

B.2 Key objectives and expected results

- Connect to, or preferably become a partner in, the recently started Joint Mission Group Eco-design and Energy labeling (under European Technology and Innovation Platform PV WG5), in order to play a role in the formulation of EU strategies with respect to sustainability of photovoltaics
- Develop a TNO research agenda for recyclability and eco-design of Building integrated PV. Develop calculated scenarios for strategic explorations for PV in built environment, also based on the TNO reliability findings
- Promotion video à Visibility of combined approach and knowledge positions within TNO

Intended new partnerships and follow-ups

- Develop externally funded partnerships on concept development for eco-design of integrated PV
- Ideation challenge proposal on Recycling of integrated PV

Body-Brain Interactions

ERP Contacts: J. Kieboom (Project Lead), R. Kleemann (Lead Scientist), P. Bongers (Science Director)

Program description

1. Problem definition

There is a need to better understand the complex interactions between body and brain because this powerful connection can be exploited to optimize cognitive and physical performance. Effective targeting of these interactions can reduce the burden of chronic and acute stress, attenuate neurodegenerative diseases and prevent a broad spectrum of obesity-associated metabolic diseases.

The ambition to optimize mental and physical fitness is timely and meets the needs of modern societies with knowledge-driven economies that require life-long optimal physical and cognitive performance. Recent demographic and socio-economic changes propel these needs and urge the development of tools and interventions to stimulate healthy body-brain interactions and to intervene in those that are detrimental.

Importantly, these interactions encompass psycho-social mechanisms as well as molecular-physiological mechanisms. The exact understanding of the integration of these two types of mechanisms is lacking and there are currently no suitable platforms available to study these interactions. This is why there are still no effective treatments for conditions such as obesity-associated dementias. Likewise, there are no effective interventions to increase cognitive performance in stressful and demanding conditions.

This ERP aims at understanding the causal determinants of both psycho-social and molecular-physiological mechanisms and at defining causal relationships to enlighten body-brain interactions that are currently still a black box. This allows the development of effective interventions. Inherent to advancing into a new field, research on body-brain interactions requires development of comprehensive preclinical (research line A) and human (research line B) test platforms to evaluate new (prevention and treatment) concepts, development of dedicated analytical and big-data science technologies for sensitive measurements, multiscale data integration and analysis as well as modelling tools for biological and psychosocial mechanisms (research line C). Research using these platforms will lead to the development of new mechanistic hypotheses and frameworks integrating psycho-social and molecular-physiological knowledge.

2. Positioning

There is little known about the exact nature of the biological signals that connect our body to our cognitive performance. Causal mediators (i.e. both chronically and acutely produced determining factors) that signal between body and brain remain largely elusive as delineated above. It is likely that certain body-derived determinants of cognitive function are critical for both chronic and acute stress situations and such generic principles are of great interest to optimize and potentially improve cognitive functioning. Also, the vast majority of research only calculates correlations between biological markers and cognitive performance without establishing causal relations and mechanistic connections. As a consequence, thereof, targeted interventions to improve cognitive performance and/or attenuate cognitive impairment are currently not possible and constitute an unmet need of stakeholders of TNO including governmental institutions and industries (pharma, nutrition, diagnostics; see ecosystem below).

It is necessary to gain mechanistic knowledge on body-brain interactions to provide effective solutions that strengthen the body-brain axis and enable people to better cope with the challenges of modern life, and to perform optimally in demanding situations.

3. Objectives and approach

The long-term goal of the ERP BBI (2023) is to understand the bi-directional interactions between body and brain and ultimately to improve human cognitive and physical performance and strengthen human health.

The program has three main research lines, each with two multi-year objectives.

Research Line A 'Preclinical Body-Brain platforms': new rapid translational models for mechanism-based preclinical research. Allowing innovative treatments that cannot be tested in humans, or tissue analyses that are not feasible in humans (e.g. analysis of brain tissue) or not practical in humans (e.g. development of dementia and other brain disorders requires decennia). Multi-year objectives:

a) to unravel the causal underlying mechanisms and involved molecular factors that signal between body and brain.

b) to test new treatments that may improve cognitive performance and attenuate brain disorders (inflammation, dementias).

Research Line B 'Acute stress human Body-Brain platforms': analysis facility for comprehensive and simultaneous measurement of metabolism, (neuro)physiology, and cognitive performance under influence of acute stressors (e.g. noise, little sleep). Emphasis is on relative rapid (acute) cognitive performance changes of a person, for instance during challenging work. Multi-year objectives:

a) to comprehensively measure different body- and brain-derived parameters (biochemical metabolic and inflammatory factors, (neuro)physiological and socio-psychological parameters) and cognitive performance parameters of a given subject exposed to one or more acute stressors.

b) to develop predictive algorithms that use these parameters to predict the cognitive performance of a person and inform on potential future decline.

Research Line C 'Chronic stress human Body-Brain platforms': knowledge platform employing advanced molecular (omics) techniques on tissues combined with Systems biology data science to assess determinants of chronic cognitive decline. Emphasis is on metabolic, inflammatory and other biological traits that determine cognitive performance and health on the long run, i.e. the biological set-points on which acute stressors of research line B are superimposed. Multi-year objectives:

a) to develop new and generic analytical & bioinformatical technologies for analyzing microbiota changes and microbiota-derived metabolites. These technologies must be generic to allow translation between the preclinical Body-Brain platforms (line A) and human platforms (lines B,C).

b) development of a new statistical method to analyze non-linear relationships between microbiota and organ histology outcomes or cognition test results (incl. non-linear correlation analysis).

The main approach of line A and line B is to perform human and rodent studies to identify key biological parameters (biochemical molecules, (neuro-)physiological and socio-psychological parameters) that determine cognitive performance and cognitive health. The main approach of line C is to analyze relevant longitudinal human datasets obtained from the collaboration with Rijnstate/Vitalys and Radboudmc/Donders (BARICO trial) and link outcomes to our own studies.

Modulation of body-brain interactions based on knowledge about underlying mechanisms has very broad applications and can solve critical challenges of modern societies (e.g. coping with multiple stressors, enhancing cognitive performance and physical fitness, reducing cognitive-metabolic disease burden, etc.). This is relevant for roadmaps *Operations and Human Factors, Biomedical Health, Child Health, Digital Health Technologies, and Work, Prevention & Health*.

At the moment 5 PhD candidates contribute to the ERP-BBI (C. Bottenheft; F. Seidel; I. Stuldreher; A. Tengeler; D. Vreeken), three of which mostly financed by our partners (e.g. Rijnstate hospitals; NWA-Neurolab; Radboudumc).

4. Applications and partnerships

The added value of the ERP for stakeholders is: a) mechanism-based understanding of the interactions; b) broad application potential (defense, police, pharma and nutrition industry, eHealth/tech-companies); c) unique TNO position because of integrated technologies that combine β/γ-expertise to efficiently improve body-brain mechanisms. Developments in research lines are in close partnership with stakeholders and partners. Current ecosystem and partnerships:

- **Academic**: LUMC Department of Clinical genetics (neuropathology), LUMC Center for Proteomics and Metabolomics, Radboudumc department of Anatomy, Donders Institute, Technical University München Institute for dementia), LCAB/Hogeschool Leiden, Leiden University, University of Ghent, University of Tilburg, University of Twente; University of Oslo, Norwegian Univ. of Life Sciences
- **Industrial**: Pharma & Nutrition (Bayer, Heel Gmbh, Ashahimatsu, Kikkoman; Norwegian Meat and Dairy Sector); Diagnostics (Nordic Biosciences, Histoindex, GBS, Quickzyme Biosciences, Genomescan); potential partners: industries that require cognitive performance in stressful situations (e.g. nightshift)
- **Governmental/NGO**: Ministry of Defense, US Airforce Research Lab, US Army Research Lab, ZonMW, Maag Lever Darm Stichting.
- **Others**: Tecnilab, Rijnstate Hospitals, Obesity Clinic Vitalys; Lowlands.

Plan Year 2021

A. Plan – Research Line A "Preclinical Body-Brain Platforms"

A.1 Key results so far

- Performed preclinical study on gut – brain interactions, analyzed effects of gut microbiota-derived mediator propionate on body and brain. Results analyzed and published in *FASEB J (2020);* establishment of prototype v1.0 preclinical model as planned in roadmap (RM).
- Completed preclinical experiment (in-life phase) on liver-brain interactions, analyzed effect of liver-derived pro-inflammatory blood factors on neuroinflammation in brain. Established method to measure this factor in blood and developed assay for humans as planned in RM. Molecular analyses ongoing for publication together with LUMC-Clinical Genetics.
- Designed preclinical study of adipose tissue – brain interactions with fMRI in collaboration with Radboudumc/Donders to establish a new link between body and brain as defined in RM. All protocols, ethical approval and mice breeding in place for start in Q3 2020.
- Awarded ZonMw grant to cover neuroimaging part of preclinical study of muscle (exercise) – brain interactions with Tecnilab & Radboudumc; results in extra PhD (new) for our ERP.
- Developed and delivered new preclinical analysis technologies (e.g. brain gene profiling) and new BBI mouse model and tissues to external partners i.e. LipidInflammaGene Consortium and other collaborations *Alvarez-Amor et al. Int. J. Mol. Sci*. and Bernhagen *et al., Nature Communic*. (both under review) -> impact goals of RM.

A.2 Key objectives and expected results

- Perform adipose tissue – brain interactions study (in life phase) and start postmortem analyses. In collaboration with Radboudumc/Donders Institute. First experimental evidence for causal role of adipose tissue dysfunction in development of cognitive decline.
- Complete analyses of liver – brain interactions study and draft and submit publication(s). Establish link between health state of the liver and the brain – potential new neuroinflammation model for pharma.
- In-depth characterization of neuroinflammation in the preclinical platform by RNA sequencing (mechanistic characterization) and DNA sequencing (genetic characterization by partner LUMC-Genetics) to provide a thorough mechanistic understanding of the new preclinical model and to substantiate the uniqueness of TNO's proprietary model.
- Investigate body-brain effects of different human diets (animal fat, plant fat jointly with LipidInflammaGene Consortium) and metabolic stressors as demonstrator for relevance of the preclinical model (e.g. food sector; optimization nutrition military personnel).
- Design and initiate preclinical study on muscle (exercise) – brain interactions. Extension of model to stroke & dementia research.
- Development and application of analytical platforms bridging preclinical and human platforms (e.g. plasma biomarkers; readouts for stressors; functional MRI imaging of brain).

B. Plan – Research Line B "Human Body-Brain Platform: Acute Stressors"

B.1 Key results so far

- Performed and analyzed experiment on cognitive, behavioral, (neuro)physiological and metabolic effects of single versus combined acute stressors: noise and skipping a meal. Conference presentation and paper submitted. *Bottenheft et al. (in revision) Effects of a metabolic and sensory stressor on cogn. task performance. Cognition, Technology and Work.*
- Designed acute sleep deprivation study: alignment with chronic study, established collaboration with Ghent University and US Airforce Research Lab. Remainder of 2020: submission to METC, building and piloting setup, start logistics and recruitment participants.
- Analyzed and wrote about (neuro)physiological and cognitive performance data under conditions of increased workload with and without acute physical threat (of an electric shock). *Van Beurden et al., Towards user-adapted training paradigms: Physiological responses to physical threat during cognitive task performance. Multimedia Tools and Applications (in press).* -> contributes to impact goals of RM
- In collaboration with Tilburg and Ghent university: extension of METC protocol to collect extra (cognitive performance and self-regulation) data in high school students in a longitudinal study. Started data analysis and publication writing on the connection between acute social stress (physiological and inflammatory responses), chronic stress and cognitive performance in high school students. -> contributes to network and publication aims of RM.

B.2 Key objectives and expected results

- Perform an integrated BBI study to identify determinants (psychological, biological and physiological factors) that predict cognitive decline upon acute sleep deprivation stress:
  - Establish the relation between cognitive impairment due to sleep deprivation and inflammatory stress response, to test the hypothesis that inflammation underlies cognitive decline.
  - Determine (neuro)physiological, psychological, metabolic and inflammatory parameters that predict

inter-individual differences in cognitive decline induced by sleep deprivation
  - Determine parameters that predict upcoming lapses in cognitive performance within an individual (-> identify early physiol. signals that signal future cognitive impairment).
  - Establish optimal methods for dynamical data analysis, enabling the prediction of inter- and intra-individual cognitive performance
- Revision to finalize the publication and analyses as mentioned in B1, 'Key results so far'.
- Submit paper with a collective of international scientists on methodological aspects of eye measurements as a tool in various research and applied domains.
- Submit a grant proposal with Leiden University for a science communication grant on opportunities and ethics of wearables in youth.

C. Plan – Research Line C "Human Body-Brain Platform: Chronic Stressors"

C.1 Key results so far

- Completed cognitive test battery, neuroprofiling and organ biopsy collection; n=125 BARICO patients as planned in roadmap (RM).
- All human tissues (organs, microbiota, plasma/serum/cells) processed and stored at TNO.
- Liver pathology (n=125) revealed that tissues are optimal, reflecting specific disease stages.
- Liver mRNA isolated and subsequent genome-wide gene expression profiling performed.
- Started metabolomics: microbiota profiling & metagenomics, amino acid profiling, fatty acid profiling (plasma & blood cells) to identify determinants of cogn.perform. as planned in RM.
- Established first joint bioinformatics infrastructure for data sharing and dedicated analyses (lead TNO, partners Rijnstate and Radboudumc/Donders)
- Establishment of an ecosystem and preparation of research propositions with the preclinical and human platforms of the ERP for: Heel GmbH, Servier Pharma, Bayer GmbH, Asahimatsu Japan, Nordic Bioscience (agreed), Maag-Lever-Darm-Stichting (transferred TKI budget), and LUMC Metabol. & Proteomics Center (scientific collaboration) to increase external impact.
- Exchange of protocol and methods for alignment of cognitive tests, biological assays between Radboudumc/Donders, DSS, HL to obtain aligned BBI platforms (preclinical & human).

C.2 Key objectives and expected results

- Identification of new links between the health state of organs and cognitive endpoints (short-/ long-term memory scores; IQ scores; etc.) and brain structure (grey matter; fMRI) using novel TNO biostatistics methods (e.g. develop non-linear correlation analysis).
- Identification of new links between health state of liver and associated disease pathways and behavioral traits (e.g. depression score; motivation score; impulsivity)
- Adipose tissue - brain interaction: histopathology (n=125x 3 functionally different adipose depots: subcutaneous fat, omental fat, visceral fat)
- Plasma profiling to identify microbiota-derived metabolites (bile acids and short-chain fatty acids) and other factors (lipids, proteins, metabolites) that mediate effects gut -> brain; adipose -> brain and liver -> brain interactions.
- Establishment of collaboration program adjacent to ERP-BBI with partners that contribute to (Gut-Liver-Brain-InterAction-Links in Obesity; GLoBAL consortia).
- Preparation of 2 papers on chronic stressors and body-brain interactions.

Social eXtended Reality

ERP Contacts: M. Boen-Leo (Project Lead), O. Niamut (Lead Scientist), P. Havinga (Science Director)

Program description

The TNO Strategic Plan 2018-2021 identifies the importance of **media synchronization**, with a focus on the combination of eXtended Reality (**XR**, the superset of AR/MR/VR), 5G and Tactile Internet. In the **ERP social XR** we aim to realize the first-time engineering of a shared and networked XR environment for **holographic communication**, where participants get the feeling of being in the presence of, and interacting with, other persons at a remote location. TNO Units DSS, HL, ICT and TT have expressed interest in holographic communication. With such a system, national security personnel (e.g. police officers) can ask for remote assistance and discuss with an expert colleague about a crime scene on location; distributed teams of soldiers can jointly train for critical missions; companies can let their personnel meet and discuss remotely, and public services offering Mobility-as-a-Service concepts can add an entire new modality to their portfolio. The output of the ERP is absorbed in VP ICT (a.o. PMCs Immersive Human Communication and Customized Digital Infratructure), and in VPs/PMCs in Units DSS and T&T. Holographic communication involves the capture, coding, streaming and rendering of spatial audio, volumetric video and tactile data. To reach Internet-level scale, cross-layer and joint **orchestration** of media, computation capabilities and network functionality is essential in a holographic communication platform. We also consider key social cues in mediated, bidirectional, multi-party interaction and key factors that make and break the experience of social presence.

1. Problem definition

Example of remote presence through holographic communication. (source: Oulu 6Genesis vision for 2030)

Transporting one's social and functional self to any place on earth is a compelling and exciting idea, providing expertise or skills at a distance e.g. in industry (co-working, inspection, maintenance), enabling remote education and training, and supporting inclusion of citizens with accessibility barriers. Enabling remote communication and collaboration provides a strong contribution to societal challenges. Examples include virtual meetings to reduce commutes, lower our economic and ecological footprint, and alleviate physical distancing measures in case of pandemics such as COVID-19. There is a strong need to make communication and remote collaboration as transparent as possible (meaning that the interface should appear to be imperceptible and almost nonexistent to the user), which can be achieved by increasing the quality of auditory and visual media, decreasing transmission delays and adding multiple sensory modalities like tactile and haptics. **Holographic communication** is such a future form of mediated social communication that enables collaboration and shared experiences. It has the promise to make this idea come true but they depend on breakthroughs in creating fast and open network infrastructures, in blending the digital and physical worlds into a multisensory, immersive world, in empowering edge devices, and in sensors and actuators for immersive multisensory telepresence. These build on current developments in 5G, Tactile Internet, Artificial Intelligence, and Augmented and Virtual Reality, (AR/VR) and together create new possibilities for communication and communication towards an era in which human capacities are supported and enhanced by an Internet of Abilities (IoA).

2. Positioning

Within TNO, we build upon an existing web-based platform for 2D video social VR experiences. ERP results feed into new modules (e.g. the MCU), or updates of existing modules (e.g. updated capture). We further build on knowledge about static network slice creation and cloud deployment of platform functions to realize an adaptively tailored network slice for the resource/cost-efficient and QoE-effective support of application scenarios. Building on earlier research into mediated communication, our human factors research focusses on required social XR system capabilities for specific use cases, and provides guidelines on how to implement social cues in social XR.

Compared to developments outside of TNO, we aim to be unique in i) our efforts to develop modules for real-time volumetric capture and rendering of humans; ii) integration of haptic / tactile interaction; and iii) delivering network supported quality through distributed processing and optimized radio connection to and from the network edge.

3. Objectives and approach

ERP Social XR consists of three research lines, and collaboration and project management activities.

- (RL1) **immersive technologies:** full end-to-end immersive experience workflow, including volumetric video and tactile/haptic data;
- (RL2) **empowered edge:** adaptively tailored 'Social XR' network slice for resource/cost-efficient
- and QoE-effective support of application scenarios;
- (RL3) **human factors and QoE:** validate the application potential of the technology and determine technical requirements and generate new knowledge on human factors.

While we treated these topics in parallel in 2020, we have planned integration of empowered edge devices into immersive experiences for holographic communication in 2021 and beyond.

4. Applications and partnerships

We have submitted multiple joint project proposals that enable partnerships and generate co-funding:

- Involvement of, and collaboration with multiple MSc / PhD students at TU Delft;
- Submitted H2020 proposal 'SUPERNOVA' with a.o. Siemens, Samsung, Orange and Telenor;
- Submitted NWA proposal 'Approaching 0' with a.o. TU Eindhoven, Twente University and TU Delft;
- Submitted ZonMW IMDI proposal on Telementoring assisted by augmented reality with University Medical Center Utrecht, Intuitive Surgical Inc., and several healthcare institutions;
- Involvement in Proeftuin op de Noordzee with TU Delft, Gemeente Den Haag, KPN, KNWV, SIC;
- Preparing collaboration with Meander Group on Corona use case 'Elderly at Nursing Home';
- Preparing ITEA proposal 'COmMunicate and collaboRAte in extenDed rEality' with KLM, KPN and the Virtual Dutch Men;
- Preparing NWO Perspectief proposal with CWI, TU Delft, Twente University and Utrecht University;
- Preparing XR meeting use case for Defense Contour programme 'Immersie Op Maat';
- Preparing pitch for Shared Research Programme with Microsoft.

Plan Year 2021

A. Plan – Research Line Immersive Technologies

Focus on designing a full end-to-end immersive experience transmission chain by focusing on two main topics: i) immersive content and volumetric video data and ii) social touch and tactile/haptic data. In 2021, the third topic on QoE is moved to RL3.

A.1 Key results so far

- **Volumetric video:** PoP / demonstrator of orchestrated automated calibration and synchronization of a networked multi-camera configuration; a full multi-user end-to-end chain is in place, enabling research areas per modules and testing platforms; improved eye contact and HMD removal; PoP architecture to facilitate testing different volumetric video compression options.
- **Social touch:** PoP / demonstrator of multi-modal synchronized experience, using 3D hand pos ition with self-view and transmission of haptic data.
- **QoE/QoS:** a minimal set of measures that maximally describes the quality of mediated social communication at different affective processing levels.
- **Dissemination:**
  - "Let's Get in Touch! Adding Haptics to Social VR". L. Fermoselle *et al.* In ACM IMX '20.
  - "Holistic Quality Assessment of Mediated Immersive Multisensory Social Communication", submitted to EuroVR 2020.

A.2 Key objectives and expected results

- **Capture and rendering:** PoC of orchestrated automated spatial calibration and synchronization of multiple users immersive content in a shared XR environment, where each user is captured with a dual camera setup as well as a tactile interaction system. The visual capture will focus on the acquisition of real-time volumetric video, investigating volumetric video formats such as 3D point clouds and light-fields. Eye contact will be improved through eye gaze tracking and HMD removal. Social touch will be expanded to reach a more realistic effect on the immersive experience. Aspects of VR and AR capture and rendering will be investigated, such as scene capture, user positioning in scene with occlusions, and AR/VR rendering devices.

- **Coding and transmission:** Low-delay compression techniques for will be investigated, which support video-based point cloud representations. The MCU will be modified to support point cloud compression with the synchronization of metadata from different sources.
- **Dissemination:**
  - o "Overview of volumetric video technologies for shared and collaborative XR", in MMSys 2021
  - o "VRComm: An end-to-end web system for real-time photo-realistic social VR communication", in MMSys 2021

B. Plan – Research Line Empowered Edge

The central objective pursued by the research line 'Empowered Edge' is the development of an adaptively tailored 'Social XR' network slice for the resource/cost-efficient and QoE-effective support of 'Social XR' scenarios, including *(i)* optimized distribution (user equipment/edge/central cloud) of accelerated media processing; *(ii)* optimized radio network deployment /management; and *(iii)* cross-layer optimization of application, processing and transmission layers.

B.1 Key results so far

- **Distributed cloud-based media processing:** the architecture of the TNO Research Cloud was amended with a GPU node which can offer both CPU-only or hardware accelerated media processing as well as serve as an edge or central cloud component, depending on a scenario. Moreover, a media processing pipeline and measurement framework were designed and preliminary automated tests to compare latencies in processing pipelines were performed. Based on quantitative measurements and experiments with realistic traffic inputs an initial blueprint of SXR slice has been delivered.
- **5G radio access:** key aspects of both the 'indoor office Social XR' use case scenarios and key 5G radio technology features have been modelled and implemented in a system-level simulator. The system-level simulator has been used to conduct extensive quantitative assessments of the feasibility, performance and capacity of handling 'indoor office social XR' scenarios over a 5G RAN, incl. sensitivity analysis wrt. e.g. scenario aspects, used spectrum, RAN deployments and radio network management.

B.2 Key objectives and expected results

- **Distributed media processing:** processes will be accelerated by pushing heavy computing methods to the edge/cloud such as point clouds encoding, image smoothing, collision detection or rendering. We generate key insights into the placement and scalability potential of the media functions, and a decision where to place SXR workloads (e.g., edge or central cloud) can be conditioned on bandwidth and latency budget and constraints like availability (or lack of) GPU accelerators. Moreover, an influence of the changing conditions like increasing number of participants or users on being in motion needs to be constantly taken into account.
- **5G radio access:** we consider more challenging scenarios involving higher numbers of participants ('massiveness') as well as device mobility. The performance/capacity potential of new radio features will be investigated, including the development and assessment of corresponding management solutions, incl. e.g. latency-based scheduling, dynamic TDD, dynamic uni/multicast and smooth distributed/multi-user massive MIMO.
- **Dissemination:** publication on the edge capabilities and placement, submitted to MMSys 2021.

C. Plan – Research Line Human Factors

In RL3, we aim validate the application potential of the technology and determine technical requirements and generate new knowledge on human factors.

C.1 Key results so far

- **Showcases:** first identification and implementations of two use case classes, i.e. XR meetings and eXpeRtise at a distance; draft document with specification of use cases and corresponding (human factors) requirements, based on interviews with stakeholders (DSS, ICT, T&T); addition of specification of 'Corona' use case on using social XR for elderly in nursing homes, with problem analysis, challenges, requirements.
- **Validation:** internal evaluation of XR meeting showcase; evaluation on depth of connection photo-realistic avatars vs graphical avatars.
- **Dissemination:** "Influence of Photorealism and Non-Photorealism on Connection in Social VR", N. Bierhuizen et al, submitted to EuroVR2020.

C.2 Key objectives and expected results

- **Showcases:** showcase updates together with external (business) partners, and identification of utility factors from end users that contribute to defining utility functions including cost, comfort, etc., the requirements of end users to satisfy their activity based needs, and the accessibility through sustainable modes of transport for replacing physical activities

- **Social presence:** determining key social cues in mediated, bidirectional, multi-party interaction and implementation of 2 key cues; determining key factors that make and break the experience of social presence through expert opinion and literature review of requirements for social presence.
- **Social touch:** exploration of cues that help ensure that the touch is perceived as given by a communication partner rather than a system.

Large-Area Ultrasound: making medical imaging safe and affordable

ERP Contacts: J.-L. van der Steen (Project Lead), P. van Neer (Lead Scientist), C. Hooijer (Science Director)

Program description

1. Problem definition

Medical ultrasound is the fastest growing medical imaging modality. Because it does not need ionizing radiation (like X-ray and CT) it can potentially also be used to image and remote patient monitoring, *i.e.*, outside of the radiology department of a hospital.

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. Image quality, in particular the lateral resolution, can be shown to improve with array size and number of elements. Mainstream 2D transducer arrays are rigid and made of small ceramic piezoelectric elements (bulk PZT). The assembly of these 2D piezo-ceramic transducers is currently an extremely complicated and expensive process, putting a practical limit to the size of the transducer array in terms of cost. We target large area arrays with >1.000.000 elements on thin, flexible substrates which, combined with novel imaging and addressing schemes, enable real-time high-quality imaging and long-term remote monitoring.

2. Positioning

Mainstream ceramics-based ultrasound transducers feature ~1000 elements, with up to 4000 elements for high-end 2D probes with pre-beamforming electronics inside the probe. Scaling in terms of probe size, number of elements and also resolution is hampered by assembly costs. Different groups follow different strategies to break this barrier:

- Arrays based on capacitive micromachined ultrasound transducers (CMUT) are fabricated using semiconductor processes on top of ~1cm^2 CMOS chips. The largest capacitive micromachined transducer array in a commercial system contains 9000 elements (US based company Butterfly), which can be dynamically grouped to form different array configurations. The physical integration of readout electronics and US transducers is advantageous in terms of signal quality and form factor (miniaturization).
- Piezo micromachined ultrasound transducers (PMUT) can be made using thin-film processes, typically at high process temperatures (>400C). A US start-up, named Exo, integrated thin-film PMUT on CMOS.chips.

We target large-area arrays with >1.000.000 elements over large area (>50 cm^2). In order to have close physical contact with the body (or in general the measured object) the arrays need to be mechanically conformable ('curved'). Today, the technology to manufacture this at reasonable cost does not exist; real-time read-out of so many elements requires novel imaging strategies and electronic addressing schemes; close physical contact with the body implies that the arrays need to be mechanically conformable ('thin and curved').

3. Objectives and approach

The main objective of this project is to develop a large-area ultrasound technology platform for high-quality medical imaging and remote monitoring. The large size of the 2D arrays will lead to higher image quality and much larger field of view. The flexible form factor enables hands-free measurements, which eliminates measurement inaccuracy due to inter-observer variability as one of the main barriers to further ultrasound adoption.

The large-area ultrasound technology fits well with the 3F Roadmap since the focus is on printed, flexible and large-area electronics, where fabrication and hybrid integration know-how developed over the past years can be utilized for a new application domain.

Our ambition is to be the go-to partner for large-area ultrasound, in terms of technology and application development, with long-term engagement of strategic partners, and spin-off creation to commercialize our ultrasound technology platform for a specific application.

To achieve this, array technology, novel imaging concepts and system-level knowhow need to be developed in parallel in order to establish a complete solution. The TNO departments Holst Centre and Acoustics & Sonar combine their know-how and expertise in this project. Acoustics & Sonar has in-depth know-how on ultrasound imaging in a wide range of applications, incl. medical imaging. Holst Centre has a strong track record in flexible electronics, originally developed for flexible displays, optical imagers and health patches. Furthermore, we envision a collaboration with Unit Healthy Living on non-invasive measurement of health parameters, possibly complemented by expertise from Intelligent Imaging on AI-assisted decision making and remote health monitoring.

4. Applications and partnerships

Large-area ultrasound is a disruptive technology. Getting to a sufficient level of maturity requires a multi-year time frame. We reached out to several experts in the medical domain. They confirmed that large area ultrasound can open up new applications in the medical domain that cannot be address today. Applications include hands-free 3D imaging, remote monitoring and multi-modal imaging to complement and eventually replace CT and X-ray as preferred imaging modalities during interventional procedures. Also, we learned that our technology not only aligns well with the future organization of healthcare, but that 'hands-free' ultrasound responds to an unmet need in the *current* clinical work flow. For example, an ultrasound patch or belt could significantly reduce the physical burden for sonographers and improve the comfort of the patient, while improving the quality of data to a level suitable for reliable AI-assisted decision making.

We are actively looking for strategic partners in medical ultrasound domain, both in academia and industry. Through previous and current collaboration in funded and industrial projects, we have established a close relationship with a number of renowned parties in the medical imaging domain (see figure on the right).

In particular, we have an active collaboration in place (STW-OTP, 2 PhD's) with prof. Eugenio Cantatore (TU/e) who is an expert on mixed-signal circuit design for flexible electronics. Through PENTA/EU project ULIMPIA we team up with TU Delft (Michiel Pertijs) and Philips on wearable ultrasound patches based on Philips' CMUT technology. Furthermore, we are setting up a collaboration with prof. Chris de Korte (Radboud UMC) who is leading the NWO-Perspectief program on new 3D ultrasound techniques to improve the diagnosis of vascular diseases (Ultra-X-Treme). Finally, we intend to engage with material partners in Holst Centre's ecosystem on acoustic coupling layers.

Plan Year 2021

Medical experts have confirmed the need for large-area ultrasound, and they explained to us that we have a long journey ahead of us. Other groups are pursuing large-area ultrasound as well, albeit with different fabrication techniques. We therefore need to expand and accelerate.

<u>It is absolutely key that we are the first to file relevant IP on system level</u> (for instance, how do we read out 10^6 elements, …) and application-specific implementations (how to retain image quality when using a flexible imager with less defined geometry?). Compared to 2020 we will significantly expand our effort here.

The ERP has, thus far, successfully concentrated on one type of array transducer technology. A substantial amount of work is still needed but we want to be the <u>first in the world to demonstrate imaging with a functional large-area US array</u> to establish our reputation and engage with possible clinical partners.

A. Plan – "Large-Area Ultrasound"

A.1 Key results so far

The first phase of this ERP (2019-2020) is best described as 'proof of concept'. In 2019 basic technology development was done, resulting in demonstration of the first printed single-element transducer operating in a medically relevant frequency range. In 2020, most effort was concentrated on demonstrating the first flexible linear array in a lab environment.

The key results are listed as follows:

- We selected the optimal transducer principle (thickness mode) and realized first devices that operate between 2-10 MHz.
- We developed a unique process for fabrication of flexible thin-film ultrasound arrays
- We filed one base patent on the novel transducer structure and fabrication process and shortlisted 4 more patent ideas

- We extended our simulation framework from discrete element in air to arrays in water
- Performance of our thin-film transducers and readout improved by factor 4000 (!) since Jan 2020, to the level required for medical imaging
- Design and realization of a 128-channel flexible linear array (first ever). Measurements are on-going.

A.2 Key objectives and expected results

In the second phase (2021-2022) we expand our efforts from transducer array to system level, thereby complementing technology development with system engineering. In fact, we believe that many aspects are fabrication technology-agnostic and we see a lot of IP in this domain (electronic integration/addressing; real-time imaging of 10^6 elements) as well as more application-specific IP (strategies to image non-flat objects using a conformable imager). By the end of 2021, we expect the following results:

Technology development and validation

- Real-time imaging array with portable readout electronics: our 2020 technology demonstrator is read out using lab equipment, for maximum flexibility. In 2021 we aim at a fit-for-purpose portable readout, which enables us to do application-specific tests outside the acoustic lab.
- First validation of our proposition in a pre-clinical setting: we will support our proposition with validation of our technology for two clinical use cases, selected with the clinical partners in our ecosystem
- Benchmarking of our technology to alternative approaches: we will benchmark our thin-film technology against assembly of pre-fabricated discrete components. We will select the shortest route to a 'MVP', i.e. 'minimum viable prototype' for a selected clinical use case
- Prototype of wearable patch using piezo components: we will work on integration of components into a wearable form factor, resulting in a prototype patch

System architecture and imaging strategies

- Feasibility and trade-offs at system level, including strategies for real-time imaging, optimal transmitter-receiver configuration, benchmarking of transducer technologies, and wearable form factor, for two selected use cases
- Demonstration of selected concept for channel reduction: addressing millions of elements while keeping the number of input-output channels low (100-200) requires novel 'channel reduction' schemes.
- 5 patent intakes on system and application aspects of large-area ultrasound imaging systems

Decarbonisation (BrightSite)

ERP Contacts: P. Winthaegen (Project Lead), A. Dortmans (Lead Scientist), C. Hooijer (Science Director)

Program description

1. Problem definition

Accelerated global warming due to the exponentially increased CO_2 emissions in the last 100 years is declared as a major societal challenge. Worldwide, governments and business communities have formulated objectives and measures to limit and reduce the emission of greenhouse gases (GHG). In June 2019 the Dutch government has formulated the ambition to reduce GHG emissions at a national level by 49% by 2030 and by 90% by 2050 compared to 1990 (Klimaatakkoord).

The Dutch chemical sector makes a high contribution (about 60%) to the total national industrial emissions of CO_2 and other GHG such as N_2O. On a regional scale, the chemical industry, located at the Chemelot site near Geleen is responsible for about 30% of the total energy consumption and 30% of the emission of GHG of the Province of Limburg. The overview in figure 1 shows the historical, current and required development of the GHG emissions at Chemelot. This shows that 2030 reduction targets can be met in principle, but that for 2050 new affordable, safe and acceptable technological options have to be explored and developed.

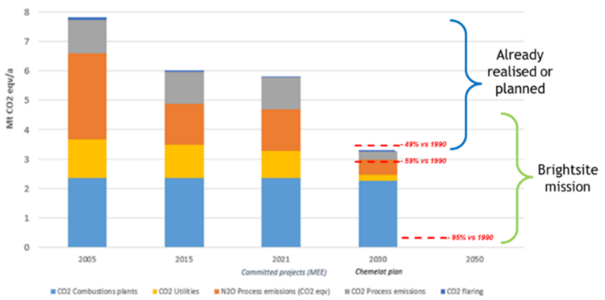

Figure 1 Origin and options for reducing greenhouse gas emissions at Chemelot

The ERP Decarbonisation focusses on the exploration and development of these new technological options and is part of "Brightsite", a shared research centre established in June 2019 by TNO together with Sitech Services, Maastricht University and Brightlands Chemelot Campus. The ERP Decarbonisation provides about 75% of the annual TNO contribution to Brightsite of 2MEUR. In the Brightsite program, also contributions from TNO VPs of the contributing units Industry, Energy Transition and Circular Economy & Environment are included ensuring a seamless integration of the ERP-activities in the strategic plan of Brightsite and TNO roadmaps.

2. Positioning

Inspired by climate change needs, a multitude of "green" technology options is pursued worldwide by academia, technology institutes and private companies at TRL 1-9, often supported by large scale regional/national/EU public funding programs. In 2019 a Chemelot system transition study was carried out during the development and start-up phase of Brightsite as part of this ERP. The study concluded that the core of Brightsite should be based on programs on **(1) Electrification**: "*Preventing CO_2-emissions related to use of natural gas for heating and production of hydrogen*", **(2) Recycling**: "*Replacing fossil carbon and hydrogen by use of (plastic) waste and biomass*" and **(3) Process Innovation**: "*Reducing emissions by increasing process efficiency or new after treatment methods*". These core programs are supported and connected by integral programs on **(4) Safety & Society**: "*Ensuring safe to apply and societally acceptable innovations*", **(5) Transition Scenarios**: *"Modelling safe, durable and economical transitions to meet 2030/50 climate goals"* and **(6) Education & Human Capital**: "*Empowering a new generations of researchers and work force*". The ERP Decarbonisation participates in programs 1-5, with focus on programs 1, 2, 4 and 5. TNO VP Industrial Transitions provides substantial co-funding for program 5 and program 6 funding is covered by Maastricht University and not further discussed here. Start-up funding of the province of Limburg, TKI-Chemistry and in kind contributions of various Chemelot companies complements the TNO ERP/VP investments, which together provide the basis for ongoing additional funding applications on generic and specific program topics. The 6 programs now firmly constitute the Brightsite program providing TNO and (founding) partners with the perspective of developing a new competitive position for comprehensive consultancy on greenhouse gas driven industrial transitions which can be exploited at international level.

3. Objectives and approach

Following the broader start up and technology selection phase executed in 2019, the ERP-funded contribution to the various programs in 2020 is now focused on:

Program (1) "Electrification": cost effective plasma technology for simultaneous CO_2-free production of hydrogen and ethylene from natural gas. This program is directly connected to roadmap Sustainable Chemical Industry of unit Industry and CO_2 Neutral Fuels and Feedstock of unit Energy Transition. Support of long term PhD research has been initiated in collaboration with Maastricht University and Differ as key science partners.

Program (2) "Recycling": at present MILENA gasification technology for cost effective recycling of plastic waste and biomass as fitting directly in the roadmap CO_2 Neutral Fuels and Feedstock of unit Energy Transition and the roadmap Circular Plastics of unit Circular Economy and Environment. PhD research is foreseen at Maastricht University and Utrecht University e.g. on next generation chemical depolymerisation technologies of mixed and contaminated plastics as fitting directly in the roadmap Circular Plastics of unit Circular Environment & Environment.

Program (3) "Process Innovation": final decision on ERP contribution to be made.

Program (4) "Safety & Society": use and processing of Health-Safety-Environment (HSE) data and other process data available at company and site level by a dedicated Artificial Intelligence (AI) model to ensure safe and acceptable future operations. The model will provide early warning information for the possible occurrence of incidents on operation of present and future process technologies (such as plasma technology or chemical recycling mentioned before). Also the AI model will contribute to the overall equipment effectiveness (OEE) and resource efficiency. This development fits in the roadmap Industrial Safety of unit Circular Economy and Environment. PhD research is foreseen at University of Amsterdam.

Program (5) "Transition Scenarios": modelling future transition pathways that are cost effective, safe and socially acceptable to support decision making by stakeholders on the transition of Chemelot. A comprehensive mathematic Chemelot site model, including modules for specific subprocesses and interrelations will be the central vehicle allowing full scale transition simulation for "stress testing" of present and future material flows, energy/heat balance and infrastructure. This fits in the roadmaps: "Towards a reliable, affordable and fair energy system after the energy transition", "Towards CO_2 neutral industry" and "Towards broad support for the energy transition" of unit Energy Transition. PhD research is not yet initiated but is expected to be established with already involved groups of Maastricht University, Delft University of Technology, Utrecht University and Radboud University Nijmegen.

A Brightsite Scientific Committee has recently been installed to provide support in setting-up scientific networks and projects and provide scientific feedback and advice. Present members are: prof. Maarten Honing (UM), dr. Paul Brands (Brightlands) and dr. Ardi Dortmans (TNO). Because of the complexity of the required transition and the different technology pathways, the scientific scope of the ERP Decarbonisation is too wide for the single lead scientist. To this matter support is provided by a multidisciplinary TNO program team. The connection to the general Brightsite management is covered by strategic planner/TNO-liaison Dick Koster. TNO-program managers have been recruited and appointed who lead or take part in Brightsite multi-partner (program) teams: (1) ing. Hans Linden/dr. Ando Kuijpers, (2) drs. Patrick Aarts, (3) dr. Jaap Vente, (4) dr. Johan van Middelaar, (5) dr. Wouter Wetzels. In specific science areas various TNO senior/principal scientists such as dr. Norbert Koster, dr. Jan Harm Urbanus and prof. dr. Bob van der Zwaan provide additional scientific support/academic networks.

4. Applications and partnerships

The ERP-funded efforts are focused on the development, scale up and demonstration of existing and new technologies and contribute to the mid TRL scientific core of the Brightsite programme. They must provide both "climate proof" as well as economically applicable alternatives for presently applied processes which are mainly responsible for the GHG of the chemical industry at Chemelot, the Netherlands and beyond.

Program (1): Electrification. Natural gas based heating furnaces presently used to achieve the high temperatures required in naphtha-cracking furnaces by SABIC is responsible for 15% of the total GHG emission of Chemelot. When sufficient green electricity would become available, this could be prevented by a transition towards electrical heating for which basic technology is available. However in view of the associated long term and billion scale investments, SABIC (and global competitors like Shell, Dow and BASF) are all looking into this issue at corporate level. As a result SABIC Chemelot is not allowed to invest or make commitments in this field for the foreseeable time. Following the completion of the feasibility phase, it was therefore decided to put the TNO-efforts in this area on hold. The TNO-efforts in program 1 are therefore now fully focused on development of a CO_2-emission free alternative process for the current production of hydrogen through conversion of natural gas by Steam Methane Reforming (SMR). At Chemelot, OCI-Nitrogen produces hydrogen by SMR for the production of ammonia, which is responsible for 30% of the total GHG emission. Plasma technology has been shown capable to produce both hydrogen as well as ethylene from various hydrocarbons with a main focus on methane. This has drawn the interest of SABIC, since this may lower the need for intake (and costs) of naphtha and provide a climate proof and economically applicable solution for conversion of methane which is extensively formed and burned at present during cracking of naphtha. Maastricht University has meanwhile committed a substantial part of its resources to program (1) by appointing a new full plasma chemistry professor (Gerard van Rooij, Differ) and providing an investment budget for recruiting of additional personnel and setting up a plasma technology lab at Chemelot in collaboration with TNO. A 2nd stage NWO-Perspectief proposal for funding of 10 PhD positions at Differ, Maastricht University, NWO, Eindhoven University of Technology, Radboud University Nijmegen and University of Twente will be submitted early September 2020.

Program (2): Recycling. Until now the TNO ERP-efforts in this area have been mainly focused by investigating and supporting the position in the field of gasification of TNO joint venture Synova. In the feasibility phase the commercial application possibilities and competitive edge of the underlying Milena/Olga technology have drawn the interest of possible end users OCI and SABIC. In specific product domains such as, recycling of Nylon, PVC and rubbers, additional Chemelot stakeholders like AnQore, Fibrant, DSM, Vynova and Arlanxeo have become involved and are additional potential partners for these developments. This calls for further investigation into the present robustness and possible flexibility of the Milena/Olga gasification technology. In view of this positive outlook, Synova is completing discussions with investors to be able to build a 10 kton demonstrator plant at Chemelot. In addition to gasification, possibilities for development of alternative recycling based on pyrolysis, chemical dissolution or depolymerization technologies are considered. Additionally, the conversion of biomass is considered. Potential collaboration with partners new to Chemelot like BrigH2 and Vertoro can be mentioned. Maastricht University has reserved budgets to set up a dedicated science group in the recycling area and contacts. In addition, PhD based collaboration with the scientific group of Bert Weckhuysen (Utrecht University) will start and be expanded into joint project proposals as in NWO Perspectief.

Program (3): Process Innovation. Options for reuse of residual heat, CO_2 capture/storage/use, treatment of N_2O and other effluent gases were assessed during in 2019 and 2020 with various industrial partners. So far insufficient industrial commitments have been encountered to start a dedicated program in this broad field.

Program (4): **Safety and Society**. In this area the ERP efforts have been focused on the development of an AI-based tool to provide a way out of the present stand still in controlling and lowering the occurrence of incidents at Chemelot and the broader chemical industry. The tool looks for hidden patterns in existing HSE, company and site data to detect early warning signals and precursors to imminent incidents. This has drawn the interest of AnQore, producing highly toxic cyanide-based compounds at Chemelot. Based on this example additional interest has led to interactions at SABIC, with the VNCI and Safety Delta Netherlands and EU-look-alike organisations (such as the European Process Safety Centre, EPSC) to discuss the application potential partnerships and support from the wider (chemical) industry field. Various academic contacts have been established in the AI and related complexity field to develop (funding for) PhD positions to support the further developments (Amsterdam University, Maastricht University).

Program (5): Transition Scenarios. This program builds on a previous analysis made by the Chemelot Sustainability Team coordinated by Sitech before Brightsite was formed. By adding and extending related TNO positions in this field a comprehensive mathematical model of Chemelot and its surrounding has now become available to stress-test the effects of various possible changes to meet the 2030/50 emission targets. For this TNO supplied expertise on circular economy, policy, external developments and behavioural science. In view of the relevance for the wider scope of the TNO VP Industrial Transformation set up in 2020, alignment and co-funding of the efforts in this area has been established recently. This provides possibilities to extent the Chemelot-based model to the situation look-alike situations and needs such as Moerdijk and Europort.

Plan Year 2021

The process for establishing the Brightsite year plan 2021 took off in July 2020 with a Steering Group review meeting with representatives of TNO and the other Brightsite partners. This process will be finalized in November, in parallel and in alignment with the TNO ERP decision making process (incl. KIP). The input from the ERP Science Board review will be included to guide the broader Brightsite year plan 2021 process.

A. Plan – Research Line (1) “Electrification”

A.1 Key results so far

TNO positions and ideas in the field of electric naphtha cracking, molten metal and plasma-based hydrogen production have been investigated and reviewed with industrial and academic partners in 2019 and first half of 2020. This has resulted in focus of the ERP-efforts on the development of plasma technology for CO_2-free simultaneous production of hydrogen and ethylene various hydrocarbons with a main focus on natural gas. This has the potential to open up a new and challenging but possibly highly rewarding “green” process route if successful. Based on extensive literature, patent and market reviews it has become clear that a 1st generation demonstration process could probably be built by combining existing unit operations for initial plasma-based conversion of methane to acetylene and subsequent hydrogenation to ethylene in a separate step. Based on the present outlook for development of electricity prices, efficiencies of presently applied processes and CO_2-taxation costs, the business case for large scale application is too weak, but options for substantial improvement have been identified in 2020 for realisation of next generation systems and processes (feedstock, plasma and process optimization). To host supporting academic research in this area, a dedicated "plasma chemistry" full chair has been established by Maastricht University per 01 May 2020 and the setup of a joint UM/TNO plasma technology lab at Chemelot has been started.

A.2 Key objectives and expected results

ERP-activities are oriented on the investigation of possibilities for the required optimization of the state-of-the-art electrical to chemicals conversion efficiency which determines the business case for widespread future application. To reduce energy losses, we will build on existing TNO experience, insights and ideas to create plasmas primarily at or nearby the surface of (catalytic) reactor surfaces in reactor design dedicated for this specific application. To achieve this we will focus on (1) optimisation of plasma type/control (electric arc vs. microwave, pulsation/temperature control, reactor design, electrode configuration etc.), (2) process control (feed stock composition, high pressure operation, residence time, quenching/cooling) and (3) in situ or after treatment (catalytic hydrogenation of primary products towards ethylene. Experimental (explosion proof) possibilities to investigate this latter process step safely are available at TNO Ypenburg. The final result for 2021 will be a first design of a prototype reactor (TRL 2-3) and patents resulting from that. Supporting fundamental research will come in place by projects in NWO and EC calls, as already initiated in 2020 such as the 10-12 PhD NWO Perspectief proposal, the 2020 MOOI proposal, and further proposals to be developed.

B. Plan – Research Line (2) "Recycling"

B.1 Key results so far

Based on the efforts made so far, the application of Milena/Olga gasification technology - originally developed for energy generation - to generate long chain hydrocarbons and hydrogen from polymer and house hold waste materials, has been proven to be a realistic option at Chemelot for replacement of fossil based feedstock. A study has been carried out on the suitability of various available waste streams and representative samples will be tested in the TNO-Petten gasification facilities in the remainder of 2020 to investigate the robustness and application scope of the technology for this purpose. Alongside these mainstream gasification efforts, the potential of and interest for development of alternative pyrolysis and chemical dissolution recycling processes has been discussed with various Chemelot based companies. From these, possibilities and interest to obtain a new "green" grade of pyrolysis oils by partial dissolution of plastic waste in naphtha-like media have emerged as an additional applicable option in the recycling area. Discussions with end user SABIC and the scientific group of Bert Weckhuysen (Utrecht University) supported by investments of Maastricht University to establish collaboration in this area have started.

B.2 Key objectives and expected results

In 2021 the ERP-funded efforts are expected to be focused on acquiring an in depth understanding and options for controlling the product formation in the Milena/Olga gasification process. In addition, a more detailed feasibility study is expected on the possibilities to obtain a new "green" grade of pyrolysis oils by partial dissolution of plastic waste in naphtha-like media. Finally, the start of a biomass-oriented study is foreseen, for which a Brightsite-review on the options for use at Chemelot by partner Sitech and TNO-wide positions available provides a starting point.

C. Plan – Research Line (3) "Process Innovation"

C.1 Key results so far

As planned the TNO-possibilities and ideas to use low temperature residual heat, capture, store and reuse CO_2 and mitigate N_2O emissions have been evaluated and discussed with possible Chemelot-based end users. So far little support for further development in these areas has been encountered. In contrast generic interest has been found to look for possibilities to develop new digitization and AI-options to improve process efficiency and safety.

C.2 Key objectives and expected results

A NDA with AnQore and Shell is finalized at present to allow more in depth discussion/investigation of the applicability of a catalyst system (formerly developed by TNO-Petten, and licensed to Shell) as a starting point for development and implementation of a catalytic cleaning process to deal with N_2O emissions for which no solution is available at present. Dependent on the outcome of the ongoing digitization/AI discussions a new cross-technology program line may be developed in this area.

D. Plan – Research Line (4) "Safety & Society"

D.1 Key results so far

A first working AI-model (Safety Stethoscope) is available at TNO from work in the industrial safety area. The model executes advanced data analytics and can identify of hidden patterns in large amounts of data. The model has shown to provide a basis for further development of a dedicated AI system to in order to identify deviations and to derive predictive values in order to predict the possible occurrence of incidents Key HSE data from incident reports, made available by AnQore, have shown the intrinsic possibilities and provided a perspective towards further development.

D.2 Key objectives and expected results

Additional databases will be included to detect coherent deviations from expected values indicating emerging risks. In a further step the development of dedicated AI search engines screening company and process data is envisaged. The results and possible further development have meanwhile drawn the interest of other possible users at Chemelot, the broader chemical industry and industrial safety community.

E. Plan – Research Line (5) "Transition Scenario's"

E.1 Key results so far

Building blocks already available at TNO and Sitech have been used and connected to provide basic modules. Missing and additional (sub)modules and features (like electricity capacity/price developments) have meanwhile been developed, allowing full scale testing and subsequent use to assess options and insights emerging from programs 1-3.

E.2 Key objectives and expected results

Based on the outcome of testing by feeding the model with historic realistic data available from Chemelot based transitions, further optimization will be pursued by adaptation of existing and addition of new (sub)modules. From this a model system for Chemelot will be delivered that is suitable for the analysis of new technologies and provide related scenarios and roadmaps for implementation at Chemelot. Furthermore, the applicability of the model will be extended by including present processes and emission reduction driven transitions envisaged at Europoort, Moerdijk and similar (inter)national chemical sites. The results obtained in Program 5 will also provide Input for the curriculum, internships and master studies of the education programme Circular Engineering of the Faculty of Science and Engineering of Maastricht University developed as part of Program (6).

Climate and Air Quality: Next generation model system for air quality and climate change applications

ERP Contacts: R. Dröge (Project Lead), M. Schaap (Lead Scientist), A. Dortmans (Science Director)

Program description

1. Problem definition

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 emission 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 ERP.

2. Positioning

At the European and national scale chemistry transport models provide a means to perform analyses and forecasts at a 2-5 Km resolution and an hour-by-hour basis, while accounting for atmospheric chemistry. The open-source TNO model LOTOS-EUROS is one of the leading members of the European regional ensemble within the Copernicus Atmosphere Monitoring Service, in which TNO coordinates the provision of emission information and the development of the model ensemble and satellite data assimilation. The major limitation of the ensemble performance is the fact that the emission information is static (annual maps with sector dependent time profiles). Hence, the emission information does not incorporate intrinsic dependencies on environmental (weather) conditions, gives all subsectors the same nature and does not acknowledge that temporal emission variability of the same activity can be very different within a country. As a consequence, the modelled spatial and temporal variability is too flat and mismatches for pollutants dominated by dis-continuous sources (e.g. traffic, agriculture, wood combustion) can be severe. Several studies, including ours, have highlighted the potential for improvement on aspects but a consistent framework is missing. The availability of world leading experts on emissions from transport, buildings, energy and industry enables in-house coverage of important sectors.

Operational urban scale models use Gaussian or line source models to provide dispersion in a limited number of atmospheric conditions. A meteorological year is divided into these meteorological classes to calculate annual mean concentration levels from the occurrences of the classes. Often these models are focussed on traffic only, which is also the case for the TNO US-air model. As traffic is not anymore the dominant urban source it used to be, the urban scale models do not provide an accurate or complete (annual) picture of the urban air quality. The Dutch OPS model for assessment on the national scale follows a similar plume-oriented approach, but includes all source sectors. Whilst it is relatively accurate for annual mean dispersion near a source, chemical conversions and emission variability are hard to incorporate, and give rise to large uncertainties in national scale applications.

Large eddy simulation (LES) models are developed within the scientific community to calculate atmospheric dispersion on a 1-50 m resolution. Prominent models are the German PALM and Dutch DALES systems. Where PALM has a key strength in modelling urban areas at the meter scale, DALES has been developed by WUR and TUD (with limited TNO investment long ago) to investigate pollutant dispersion including simple chemistry. So far, these models have only been used for idealized cases in the scientific community but with current computing power these become applicable to larger regions opening up the potential to address aforementioned issues in a single modelling framework at unprecedented resolution. Such a novel application over e.g. the entire Netherlands requires high-resolution, time-dependent emission information which is currently unavailable.

TNO is world leading both on the data and the instrumentation side. On the data side, the units CEE/T&T are leading in emission inventories, the modelling of air quality and the assimilation of satellite data. Coupled with instrumentation expertise from the unit IND on the development of sensor and satellite instruments, we have a unique combination of internationally distinctive know-how.

3. Objectives and approach

The overall goal 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.

A. Dynamic anthropogenic emissions– The main objective is to develop spatially (25m) and temporally (hourly) highly resolved emission data for NRT and analysis purposes. The main developments include activity modelling based on big data (IoT, AI, data mining, agent modelling) and emission behavior modelling including dependence on environmental conditions. Through these developments we will fundamentally transform the current top-down emission workflow into a bottom-up one. The emissions models will encompass air pollutants and greenhouse gases in one framework tailored to the requirements of the chemistry transport modelling systems to allow to address co-benefits.

A PhD position will be created on the use of artificial intelligence to estimate emissions (e.g. transport).

B. Hyper local air quality modelling – The main goal is to develop the Dutch Atmospheric Large-Eddy Simulation model (DALES) away from idealized scientific case studies to realistic applications for atmospheric composition. We will research the impact of the urban and rural landscape on boundary layer dynamics and the resulting dispersion of reactive pollutants. This requires accounting for anthropogenic emissions, biogenic emissions, deposition processes, atmospheric chemistry, and building resolved flows.

C. Assimilation of satellite and sensor data – The main objective is to generate objective feedback on the quality of the models and emission information. We will develop new dynamic model evaluation methods to evaluate the impact of emission and meteorological variability using recent years including the COVID-19 period. For emission verification, we will develop methods to assimilate different types of observations (satellite, sensor, instrument) simultaneously in all transport models.

D. System integration of multi-scale model system & demonstration – The main objective is to connect all components of the model system to support fast and reliable calculations for re-analyses, nowcasting and scenario assessments. In practice, a specific IT-workflow needs to be constructed which takes place from data acquisition till the provision of the insights and results of the calculations. The data management component ensures the input and output data are FAIR – Findable, Accessible, Interoperable and Reusable. Flexible integration of new data types and calculation steps is crucial. A system integration approach will be followed to ensure efficient computing and exchange of data. The applicability of the model system will be demonstrated for the greater Eindhoven area (50x50 km^2).

Roadmaps: Environment & Sustainability (emission and atmospheric modelling)., Mobility & Logistics (traffic emissions), BIM (maritime), Digitization (Urban Strategy), Space & Scientific Instrumentation (assimilation of satellite observations), ICT (system integration).

4. Applications and partnerships

A. 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 rely critically on high quality emission data.

In this starting phase we aim cooperate with national (WUR, CBS, RWS) and international experts on activity and emissions modelling. In 2020 we have submitted the EU-Enviot and NWA FORECAST proposals with TNO contributions on high-resolution emission modelling.

B. Hyper local air quality modelling with Large Eddy Simulation (LES) models will be applied 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. The main partners are TUD, VU and WUR within the framework of Ruisdael and PIP (3 postdocs) as well as the Freie Universität Berlin (1 postdoc) and Leibniz Universität Hannover (LES developers). TNO will take the lead on applications and emission information in the DALES consortium.

C. Assimilation of satellite and sensor data can be applied for verification of regional air pollutant and greenhouse gas inventories and policies. Furthermore, the optimal estimates allow for nowcasting and short-term forecasting purposes. The main (envisioned) partners are KNMI and TUD. The EU HotspotAirQuality proposal, submitted in 2020 (14 partners), focuses on the development of new sensors and the application and integration of sensor data into LOTOS-EUROS and DALES for Eindhoven.

D. System integration & demonstration will result in a model system that can be applied for assessing integrated environmental issues. It can be used for assessing 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 anticipate on a national knowledge program on monitoring nitrogen deposition with all relevant institutes to start in 2021. Later, we envisage to provide the high-resolution maps openly to allow for industry to develop services on it.

Other applications will become available when (parts of) this model system is developed, such as air pollution-adapted routing for vehicles, early warning systems for hazardous chemicals, modal shift solutions and green labeling of the transport sectors like shipping, hereby supporting abatement measures on emissions and service spin-offs for companies.

From the start 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 (e.g. I&W, LNV, UBA, Noord-Brabant, DCMR), Research institutes (e.g. KNMI, RIVM), and NGOs (e.g. Longfonds). Where possible, additional funding (matching) will be attracted to strengthen the ERP.

Plan Year 2021

A. Plan – "Dynamic anthropogenic emissions"

A.1 Key results so far

A demonstrator of the spatial and temporal high-resolution emission map of road transport has been made for 2 hours on a 5 km stretch road of the A50 north of Eindhoven. The goal was to assess the possibilities for making these high-resolution emission maps and to demonstrate the effect. These emission maps showed a large temporal and spatial variability, and it also showed that the main challenge for these emission maps is the availability and quality of activity data.

A.2 Key objectives and expected results

The key objective for 2021 is to explore and apply novel approaches to locate and parameterize the emissions of important source sectors.

The first activity will be directed to derive two base emission sets at 25 m and 1 km resolution based on spatial proxies (road networks, housing info) and existing information from the national emission inventory.

It will be researched how to use modern data analysis techniques (AI algorithms, pattern analysis) to derive activity and emission behavior models to calculate emission variability in space and time. In 2021, this will be applied on activity and emission behavior models of road transport and of households and restaurants in the Eindhoven area:

- Develop 72hr forecasting routines based on pattern analyses for household's energy use and traffic flows
- Develop predictive routines for vehicle emission behavior based on STL real world traffic emission database
- Demonstrate the feasibility of data mining to prescribe urban activities using restaurants as case study

The key results will be:

1) The static high-resolution (25m) annual base emission map for the Eindhoven area based on existing information from the national emission inventory combined with spatial proxies.
2) Novel methodologies to predict the occurrence and strength of emissions for several activities:
    a. Short term (72 h) forecasting routines for household's energy use and traffic flows
    b. Predictive vehicle emission factors including behavior and meteo effects
    c. Restaurant emission inventory based on mining Google maps

B. Plan – "Hyper local air quality modelling"

B.1 Key results so far

The DALES system as developed by TUD/WUR has been applied at TNO and standard idealized set-up was adapted for use with realistic ECMWF meteorology for Seed-ERP simulations in a 5x5 km area north of Eindhoven.

B.2 Key objectives and expected results

The key objective for 2021 is to develop the DALES system for use with realistic land use and demonstrate its application to the Eindhoven region for inert tracer dispersion.

- Develop a common space-time definition framework for DALES and the emission data
- Detail high-resolution land use maps for DALES and its process descriptions
- Perform simulations to investigate the land use impact on boundary layer dynamics and plume dispersion
- We envisage to connect the model to the static base emission set prepared in A in the third quarter and to demonstrate the concentrations for the Eindhoven area with a 25m resolution.

The key results will be:

1) DALES model version including realistic land use (module)
2) Insight in how a land use mosaic impacts boundary layer meteorology and pollutant dispersion
3) Demonstrator with 25m resolution simulations with static emissions for the Eindhoven area
4) Submission of 1 publication

Next to the technical work, we will start positioning TNO in the international ecosystem on LES initiatives and strengthen the national collaboration, via EU consortia, academic cooperation, and possible B2B leads.

C. Plan – "Assimilation of satellite and sensor data"

C.1 Key results so far

N.A.

C.2 Key objectives and expected results

The key objective for 2021 is to develop new dynamic model evaluation methods (based on satellite and sensor data) to evaluate the impact of emission- and meteorological variability for the regional scale using recent years including the COVID-19 period as testcase. We envisage that the novel dynamic emissions will especially impact the temporal variability of the modelled regional background. With this in mind, we start with the regional background in this work package.

- Quantification of the base model performance of LOTOS-EUROS for N, PM and GHG for 2015-2020
- Development of dynamic evaluation indicators and thus the regional scale evaluation strategy for further use in the ERP.
- Develop a multi-component methodology using ground based and TROPOMI satellite NO_2 data to assess the NOx emission changes during 2018-2020.
- Submission of 1 publication

Key results: Detailed insight in the dynamic behavior of atmospheric constituents as function of meteorological conditions as well as a first combined inversion of NOx emission changes for the COVID period in the Netherlands:

1) Dynamic evaluation indicators (temperature dependency, intrinsic variability)
2) Benchmark indicator set available for LOTOS-EUROS (1x1km) for N, PM and GHG
3) Method to assimilate multiple types of observations
4) NO2 distribution across the Netherlands, including parameters for model correction

D. Plan – "System integration of multi-scale model system & demonstration"

This work package will start in 2022 (delayed due to the reduction in 2021 budget).

Multi-objective Design & Decision Support for Circular Structures

ERP Contacts: A. Bigaj-van Vliet & S. Valcke (Lead Scientists), A. Adriaanse (Science Director)

Program description

1. Problem definition

On the 21st of July 2020, the EU reached an agreement on its Multiannual Financial Framework 2021-'27. Targets of the Climate Agreement and European Green Deal – **including 50% CO2 and 50% primary material reduction by 2030** – have been upheld. Financial support however to reach these targets is under pressure as the agreement is substantially affected by the Corona-related Recovery Plan for Europe. This inevitably leads to the need for setting priorities in the routes to sustainability. Enabling sustainable development is a complex, multi-disciplinary and multi-sectoral challenge with often contradicting objectives. As such, often only single aspects of the challenge are considered in innovations with insufficient information for transparent decision making and priority selection. One of the sectors currently actively experiencing this issue is **the typically fragmented Dutch construction sector. This is problematic as they are responsible for up to 10% of the total CO2 and nearly half of the annual waste in the Netherlands. As such they face a huge challenge to contribute positively to the 2030 climate ambitions.** A material with dominant impact in the construction sector is **concrete** (the largest commodity after water). This is acknowledged by the construction sector and government who launched the Concrete Agreement (Betonakkoord, 2018), additionally declaring that by 2030 all construction and demolition waste (CDW) from existing concrete structures must be reused in new concrete. The quality and performance of CDW is currently uncertain and unpredictable, so it is only used in limited percentages (only 2% of the 22 Mton/year of stony CDW, is reused in new concrete (the total Dutch concrete production is 33 Mton/year)). As a result, the concrete sector is seeking a **breakthrough in demonstrability of performance and risks of using CDW within the multi-objective context of sustainability,** otherwise their goals may not be reached[3]. Next to concrete, other materials within the building stock have high impacts on annual waste volumes. Steel is one of those, although recycling in new steel is more common than for concrete. Another pressing and ever growing issue concerns the large volumes of wind turbine blades that are facing landfill after only one 25 year lifecycle.

2. Positioning

Positioning on multi-objective optimization for sustainability (people, planet, profit)

While in recent years, computer-aided and algorithm based multi-objective design came in use in several industries to objectivize decision processes (using scatter plot diagrams, parallel coordinates, self-organizing maps etc.), it has never been developed for the complex multi-objective issue of sustainability (people, planet, profit). Specifically for engineering of (concrete) structures the decision making steps are far from being objective and are often done with rudimental methods of step-wise sub-optimization. TNO ET (AG) has solid knowledge of the modern computer-aided engineering procedures[4] to enable a unique step towards a transparent tool for *simultaneous* optimization of structural safety as well as environmental and economic performance. For this, an evaluation framework with a set of new generation design criteria and parametric models linking supply (CDW) quality to performance needs to be developed and expanded to the material level. TNO BI&M (SR) has a leading position in setting design objectives (criteria) and modeling of reliability of concrete structures[5], while TNO CEE (CAS) has a leading position in environmental impact assessment and modelling of processes and products. At the same time, this approach allows to include TNO CEE's ambition to develop dynamic – scenario based – life cycle assessment (LCA) methodologies that are better equipped to assess future environmental impact than the current LCA methods based on historical data. Also, the new approach in which supply quality (uncertainties) will be quantitatively linked to performance, will help in developing a set of circularity indicators based on the value related to technical performance or energy needed to bring used materials to their original functional quality (e.g., structural performance).

Positioning on use of existing building stock

Various techniques for dismantling and recycling currently in use or being developed, result in variable supply qualities, also depending on the origin of the concrete. Currently, no systematic quality diversification is made

[3] Letter of Jaqueline Cramer on behalf of the 'Betonakkoord' to directors of Ministries IenW, BZK, EZK. d.d. 12-06-2020
[4] Fonseca R, Reynolds A, Jansen J. 2016. Generation of a pareto front for a bi-objective water flooding optimization problem using approximate ensemble gradients. J Pet Sci Eng 147, 249–260
[5] Slobbe, Rózsás, Allaix, Bigaj-van Vliet. 2019. On the value of a reliability-based nonlinear finite element analysis approach in the assessment of concrete structures. Structural Concrete 21.

and parametric models relating quality data (uncertainties) to performance are missing, simply because the need for higher replacement levels was not yet urgent and because the market is reluctant to invest in quality improvement as long as risks and benefits are not clear. This hampers commissions in which TNO SR takes part, in trying to regulate upscaling of higher percentages of concrete recycling (e.g., TNO participation in CROW commission N1482 2019-20 'Nieuwe Recyclingmethode voor Toeslagmaterialen'), in particular for structural concrete. To overcome this deadlock, TNO SR has the expertise to develop the structural and material performance models based on measurable quality parameters, needed for sustainable design optimization. Also, TNO SR has the theoretical background to develop high performant binder blends with (organic) additives to disclose the maximum potential of CDW as well as to use reclaimed glass fibers from wind turbines (with TNO ET (WE)) for optimum concrete performance. This results in higher, quantifiable technical value as well as cost benefits.

3. Objectives and approach

The multi-year ambition is **to enable 100% reuse of the existing CDW stock while simultaneously reducing 50% CO2 and primary material use in new concrete. The overall research goal is to develop methods, models & tools for sustainability-oriented and supply quality based, multi-objective (conceptual-to-detailed) design of structures, allowing for simultaneously reaching optimum in social wellbeing, environmental impact & economic performance.** Structural safety is an explicit criterion for the social well-being aspect of sustainability in this ERP. The major highlight of the feasibility study in 2020 is the demonstration of a preliminary optimization tool including realistic but simplified parametric models linking CDW quality to performance. There is room for more criteria and complex parametric models and further improvement is possible for including uncertainties and analysis for decision support. Also, labscale mortars showed feasibility of at least 50% cement replacement by ultrafine CDW, contributing to 50% CO2 reduction. This gives us confidence to organize the full ERP along 3 research lines [RL] with feasible objectives to develop tools, models and methods for respectively:

[RL1-TNO AG, SR]Multi-objective optimisation & decision support for design of sustainable structures including uncertainties in supply quality via parametric models; **[RL2-TNO SR, CAS, WE]**New generation quality-based parametric performance modelling (structural, environmental, economic); **[RL3-TNO SR, WE]**Quality enhancement and key (in-line/in-situ measurable) quality parameters for >50% cement replacement by CDW**.**

The approach to ensure tangible research progress and implementation is to select use cases by stakeholders active involvement (see par. 4) and to include at least 2 PhDs (see Plan 2021). TNO has expertise on multiple disciplines to act as 'system engineer' as well as innovator to this complex multi-objective sustainability issue recurring in multiple *roadmaps* (Buildings & Infrastructures (Sustainable Built Environment)), Circular Economy (Next Generation Impact Assessment), CO2 neutral fuels & feedstock (Multi-objective Design Optimization under Uncertainty) and Large-scale generation of Wind Energy (Circular Solutions for Wind Turbines).

4. Applications and partnerships

The building sector, government and knowledge institutes recognize the need for a chain approach to reach full sustainability and organized themselves within the 'Betonakkoord' and 'BTIC Circulaire Bouw'. It is our active involvement in these bodies and the fundamental questions the sector faces that led to this ERP proposal. It is not the aim to develop the design optimization tool for just one stakeholder, which would hamper the envisioned chain integration. Rather, our aim is to make the tool flexible, transparent with quantified gains and risks and to include decision support from various perspectives of stakeholders (engineers, recyclers, contractors, owners etc). The resulting impact of this approach is to help the whole chain in well-found prioritization to optimal sustainable solutions to reach 100% reuse and 50% CO2 reduction in 2030. Also, the research will lead to 'spin-off' applications, which in 2020 brought commitment of academic and commercial frontrunners to be involved in the ERP (see Plan 2021). Specifically, TU Wageningen, world-class in biochemistry, and recycling company TweeR, frontrunner in ultrafine CDW separation, are involved to provide tailored additives and CDW with intended in-cash contribution via BTIC umbrella (RL 3). TU Delft Civil Engineering is involved in planning of a PhD on parametric structural performance modelling (RL 2) as well as in the multi-objective optimization tooling (RL 1). The Recycling Lab of TU Delft is the planned partner for a PhD on modelling and quantifying circularity indicators (RL 2). RWS as an owner gives expert opinion on decision support by the multi-objective optimization tool (intention in-cash via BTIC umbrella) (RL 3). Lagemaat (contractor) provides the boundary conditions for scoping the use case of reclaimed slab elements. As the complexity of sustainable design equally exists in other domains, we will reach out to those domains also involving structural safety (e.g., steel structures, wind mills).

Plan Year 2021

A. Research Line "1. Multi-objective optimization & decision analysis for sustainable structures"

A.1 Key results so far

In 2020 the technical, societal, environmental and economic performance aspects were evaluated simultaneously during the simulated design process using adopted tooling for multi-objective optimization and decision support. In particular, suitability of state-of-the-art methods to multi-objective optimization under uncertainty for sustainable design of concrete structures was assessed, with as reference the multi-objective optimization tools TNO EVEREST and open source jMetalP. 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 increasing complexity of models and include risk-awareness in decision making.

A.2 Key objectives and expected results *(TNO AG & SR)*

This research line aims to deliver a transparent design framework for multi-objective optimisation & decision support for design of sustainable structures, including uncertainties in supply quality via parametric models. The design process for any complex system with uncertainty is often executed sequentially, honoring different types of constraints covering both the supply-driven design and demand-driven supply. The developed optimization framework will use models that evaluate the parametric performance of sustainable structures designed with reused materials. A variety of different objectives (often more than 5) will be taken into account at different stages in the design process. When dealing with such a larger number of objectives, efficient algorithms need to be developed to obtain multiple (Pareto optimal) design solutions. This provides a rigorous framework for a decision maker to select from a range of optimal solutions. The interpretation and visualization of such Pareto fronts is not trivial and will therefore be investigated. To enable the efficient design of the system and exploration of the decision space we will investigate the use of Decision Trees to enable the incorporation of expert judgement into the optimization framework. The essential results foreseen for 2021 are:

- a comprehensive modeling framework for design of sustainable concrete structures made of regained materials, which includes quality data & uncertainties via an integrated value model.
- the development of a sequential chain of model based optimizations with Decision Trees which will account for the known uncertainty, constraints & expert judgement.
- the development of algorithms and interpretation for multi-objective optimization and decision support under uncertainty for cases with large number of objectives (>5). (Partner: TU Delft, CiTG & Applied Mathematics faculty, O. Leeuwenburgh and Prof. A. Heemink)
- demonstration of use case of multi-objective parametric design of concrete and composite structures.

B. Research Line "2. Quality-based performance modeling for sustainable structures"

B.1 Key results so far

In 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 modeled preliminary. 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. Next, a preliminary approach to account for circularity and reuse has been included in the environmental models. For demonstrating the feasibility of the multi-objective optimization, a case study was defined and performance models selected, and the optimization process was formulated with limited parametric variability. This is mainly because S-o-t-A models for structural, environmental and economic performance appeared insufficiently oriented to reuse, circularity and to inclusion of uncertainties. These results are convincing that the ERP can enable a major breakthrough (using parametric models for linking supply quality & uncertainties to performance). Collaboration has been established with the University of Barcelona (Prof. A. de la Fuenta) with regard to defining sustainability framework for buildings and infrastructures.

B.2 Key objectives and expected results

(a) Structural performance models *(TNO SR)*:

The aim is to develop a digital material twin for concrete based on CDW and to couple this to numerical models of the structural behavior in order to reduce the uncertainty originating from the variability of the CDW quality and to set optimization parameters for quality enhancement. The digital material twin will predict the concrete properties through an advanced model of the stress state redistribution between the cement paste and the aggregates. In order to contribute to a solution for wind turbine blades, the digital twin should also predict the performance of concrete with reclaimed glass fibers as such giving recommendations on feasibility and optimal glass fiber geometries to be reclaimed from the composites. Attention will also be given to uncertainty quantification & uncertainty treatment in data enhanced structural design aiming at establishing the link to state-of-the-art recycling and quality measurement technologies. Expected results in 2021 are:

- initiation of a PhD on digital material twin for CDW-based concrete integrated into structural failure modeling in reinforced concrete structures (partner: TU Delft Civil Engineering, Prof. B. Sluys)
- a framework to assist in setting material reliability requirements and efficient test protocols for CDW based on uncertainty quantification in structural design and to assist in data-enhanced structural design incl. use of Value of Information (VoI) workflows. (partner University of Barcelona (Prof. A. De la Fuente)

(b) Environmental performance models *(TNO CAS)*

The first aim is to enable a breakthrough in the development of prospective life cycle analysis (LCA) to take into account size scaling, synergy, and learning effects from innovations towards industrial production (currently LCA is based on static, historic data). The second aim is to develop robust uniform indicators for circularity. Two approaches will be investigated: (1) entropy-based environmental impact modelling accounting for circularity by comparing and optimizing energy levels for bringing materials back to their desired (original) performance and (2) quality-oriented residual value modelling related to material performance indicators to be included in the overall environmental impact whilst simultaneously providing input to the economic balance of the optimization.

- development and verification of quantitative general circularity indicators applicable and verified for concrete structures. (PhD at the Recycling Lab TU Delft - Francesco Di Maio)
- development and verification of a prospective LCA methodology (partner: University of Nijmegen).

(c) Economic performance models *(TNO WE)*

The objective is to expand the current simplification of cost-models as used in the 2020 feasibility study to include the whole life cycle including production, logistics, maintenance as well as end-of-life. This is particular expertise of TNO WE for wind turbines, which they will further develop for generic applicability with a focus on design aspects of 1) recyclable material combinations, 2) joining / separation technologies and 3) minimization of production waste for wind turbines. Expected results for 2021 is a working first version cost-model that is fine-tuned for structural concrete.

C. Research Line “3. Quality enhancement of secondary materials for sustainable structures”

C.1 Key results so far

In 2020 a molecular approach was formulated to design concrete binders based on CDW as such replacing an empirical approach. This 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 Ca-release is critical and requires organic additives. It is concluded that Ca/Si & zeta potential can be included as modelling parameter in design for Ca-regulation. This shows 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.

C.2 Key objectives and expected results

The objective is to develop theory and methods to determine required critical dosages for blending of organic /inorganic additives with CDW needed for disclosing the CDW’s maximum potential and to enable increased cement replacement levels higher than 50% (state-of-the-art is at 10%). This will be done by making use of material characteristics as the zeta-potential as well as Ca/Si (Al) ratio as a key parameter in dosage for binder design. It will be investigated whether these particular parameters in future can be included in the digital concrete material twin to be developed in research line 2. Collaboration will be continued with TweeR for input CDW material optimization as well as with TU Wageningen (via BTIC) and TNO B&EE for input organic additives. The results 2021 are :

- Measurement tool for quality parameters to regulate optimum dosages *(TNO SR)*
- Lab scale prototype of mortar with minimum 50% CDW in binder, regulated by (in)organic additives *(TNO SR)*
- Preliminary verification test of reuse of glass fibers reclaimed from wind in concrete turbine blades as modeled in RL2 *(TNO SR & TNO WE)*
- Feasibility of CDW quality measurement, classification & control incl requirements for (in-line) sensing for CDW mix rubble and requirements for (in-situ) assessment of remaining service life of components *(TNO SR)*