PPP programme allowance 2016

Print Drying of Suspensions - TNO (CHEMIE.PGT.2016.013)
Drying is an important production step in modern industry consisting of solvent removal from a solid or liquid phase. Today many industries, among them pharmaceutical and paper, use drying in order to reduce costs related to transport, storage, dosing and prolonging of the products shelf life.

Ubiquitous in the pharmaceutical industry there is a growing need for specific controlled dosing in medical therapy applications. It is crucial then to be able to dispense drugs controlling their composition with high accuracy. This is achieved by producing polymer particle carriers as reservoir for a given active ingredient. That carrier defines the drugs release behaviour inside the body. To obtain a narrow and controlled particle size distributions TNO's proprietary technology for high viscosity printing can be used in the production of monodisperse droplets during drying.

In here the main aim was to generate better understanding of the process and particle relation during production via drying of monodisperse droplets. Experiments are combined with the help of process simulation to determine the main factors that influence the resulting particle size distribution.

Among the results in this project it was possible to realize single droplet tracking thanks to a new visualization setup taking advantage of a telecentric lens. In parallel a numerical model and computer simulations representing the drying column and droplet injection were built. It was observed that the air flow through the drying column was not laminar with droplets dragging the surrounding air significantly. Taking such effect into account numerical calculations could account for collisions and coalescence of particles. The collisions among the particles are highly responsible for the wider size distribution and loss of accuracy. Therefore it has been suggested a new mechanism for ejecting droplets in patterns that could spread them from the start guaranteeing that such collisions would no longer occur.

Nanotechnology for early cancer diagnostics – Twente University (CHEMIE.PGT.2017.001)
Methylation of genes is a normal process that occurs in the human body and it is a process to (de)activate genes. However if this occurs for tumor suppressor genes, it can leads to the development of cancer. In this project the aim was to develop a microfluidic sensor for the early detection of cancer using urine. We found at the the presence of hypermethylated DNA in urine can be used to detect specific types of cancer. Furthermore we developed a method to extract this type of DNA from urine, by choosing an optimal density of capture molecule on the surface, thereby enabling enrichment of hypermethated DNA. This DNA can be detected using different optical or electrochemical sensors; and microfluidic chips for this have been developed.

Nano-enabled Foil Technology (NeFT) – TNO (CHEMIE.PGT.2017.003)
Thermoplastic polymer foils are key elements of many market-relevant laminates, such as safety glass, building glazing or solar panels, where they serve as interlayers for, e.g., safety- or mechanical fixation purposes. Unfortunately, such interlayers feature no optical function as such. Their only 'optical role' is to simply maintain the transparency of the laminating glass and, hence, in this sense they are optically-passive elements. The development of optically-active thermoplastic polymer foils and laminates has been identified as an important innovation field with a broad market impact prospect.

The objective is to develop a solid knowledge basis for the successful design of thermoplastic polymer foils (materials) with the right optical functionality, that is, with tailored optical characteristics (refractive index)

and optical performance for deployment as interlayers of market-relevant laminates, namely, glass- and solar cell laminates. As thermoplastic polymer we have selected polyolefins (POEs), more specifically low density polyethylenes, due to their high market relevance and outstanding chemical and physical properties, even though the knowledge that will be developed in this proposal is expandable to other thermoplastic polymers as well (e.g., polyvinyl butyral, polyethylene terephthalate, ethylene-vinyl acetate, etc.). We will bring optical added value to POE foils by incorporating optically-active inorganic nanoparticles (NPs) so that the obtained NPs-POE foils and laminates thereof feature a tailored higher refractive index and optical performance with respect to their NP-free counterparts.

The project successfully proofed the proposed principle that the efficiency of solar cells can be improved by the incorporation of selected nanoparticles into the polymer encapsulant film. We also generated an optics model to predict the obtained optical effects as a function of properties of the basic materials used. We successfully validated this model with experimental results.
We also found that the polymer encapsulant films with the large amounts of incorporated nanoparticles changed their melting viscosity and visco-elastic behavior strongly, which affected their processability on state-of-the art lamination machines.

Liposomal targeting of dendritic cells in human skin using hollow microneedles – Leiden University (CHEMIE.PGT.2017.004)
In this project we develop a new way to administer allergy vaccines and to make the vaccines more effective. Current vaccines are administered by multiple injections over a period of years. These injections are often experienced as unpleasant, causing many patients to drop out prematurely, which has a negative effect on the effectiveness of the vaccine. That is why we are going to administer the vaccines with a new painless method based on very small microneedles and the effectiveness is being studied. We will also make the vaccine more effective by targeting delivery to specific cells in the skin. In this project we show that the method of injection has a major influence on the delivery of the vaccine in desired cell lines, bringing allergy vaccine delivery using these small needles one step closer.

Synthesis of catalytic metallic and bimetallic nanoparticles by cathodic corrosion – Leiden University (CHEMIE.PGT.2017.005)
No useful summary for the general public

Powder Coating on Plastics and Composites – Windesheim (CHEMIE.PGT.2017.006)
Powdercoating on metal was developed in the 40's and 50's. Metal is conductive and can easily be heated to high temperatures like 230 °C to initiate the cure of powdercoatings. In search of a more energy efficient powdercoating process, in recent years a new generation of powdercoatings was developed, the so-called 'low temperature bake' powdercoatings. This opened up the possibility to apply these no-emission coatings on plastics and composite materials without the risk of the plastic parts melting or warping.
Using low-bake powdercoatings to coat plastic is a major step forward in the current coating processes. First of all it means no chemical steps are needed anymore, like primers, but it also opens up the possibility to coat plastic parts produced from recycled plastic material. Very often these objects show small imperfections on their surface area, making them less attractive to consumers. A very thin layer of these coatings can mask these imperfections and therefore further market acceptance of recycled plastic material. In previous research it was shown that a thin layer of powdercoating on plastic parts posed no threat to further recycling.

Within this project powdercoating was applied to thermoplasts but also to thermoset composite materials. The current coating system of for instance yachts and windmill blades emits 'volatile organic compounds' . A powdercoating system is capable of cutting that harmful emission by half.

Bifunctional zeolite catalyst for hydrocarbon conversion – Utrecht University (CHEMIE.PGT.2017.007)
"Bifunctional catalysts for the conversion of alkanes contain metal sites and acid sites. For a long time, the intimacy criterion “the closer the better” has been widely accepted for designing bifunctional catalysts. However, restricted by the lack of material synthesis and characterization methods with nanoscale precision, deep understanding and further development of the intimacy criterion is still challenging.
In this project, we select two one-dimensional zeolites (HZSM-22 and HMOR) together with alumina binder for constructing bifunctional catalysts. We selectively deposit Pt particles either on alumina binder or in the micropores of zeolites. The Pt-on-binder catalyst provides nanoscale proximity between Pt particles and acid sites, while Pt-in-zeolite catalyst gives the closest proximity. The catalysis results show that the closest proximity between Pt and acid sites is detrimental for alkane conversion. First, when employing HZSM-22 with 10-membered ring channels, embedding the Pt particles in the channels may bring diffusion limitation for alkane feedstock. Even worse, the desired isomers are prone to be cracked in the long narrow channels. Thus, the closest proximity not only causes lower activity, but also more side cracking reaction.

Comparatively, for the Pt-on-binder catalyst, the diffusion of alkane feedstock from gas to Pt sites is fast, and alkene intermediates can diffuse through alumina binder to acid sites, where they immediately undergo isomerization in outer zeolite layers and rapidly diffuse back to Pt sites. Therefore, Pt-on-binder catalyst shows both higher yield of desired isomers and higher activity. For HMOR-based catalyst, the activity of alkane conversion is not sensitive to where the Pt sites are. However, deep embedding Pt particles in the micropore channels also cause consecutive cracking of C7 isomers.

New Insights in the working principles of tri-ethyl boron as co-catalyst in Cr/SiO2 Phillips catalysis – Utrecht University (CHEMIE.PGT.2017.008)
The Cr/SiO2 Phillips-type ethylene polymerization catalysts is one of the three workhorses in catalytic ethylene polymerization. Even though this catalyst does not need a co-catalyst, these are often added as metal-alkyls for scavenging poisons, removing the induction period, enhancing the reaction rate and tailoring polyethylene (PE) properties. In this work we investigated the effect of tri-ethyl boron (TEB) and tri-ethyl aluminum (TEAl), as metal-alkyl co-catalysts, on the density of the early-stage PE materials by means of Scanning Transmission X-ray Microscopy (STXM) as a synchrotron based nano-(spectro-)microscopic technique.
Our results have shown that the density of the early-stage PE materials is affected by the type and amount of co-catalyst. The early-stage PE materials produced with TEAl were slightly less dense than those with TEB. Bulk characterization techniques revealed that this is likely attributed to the enhanced degree of Short-Chain Branching (SCB) with TEAl while the Molecular Weight Distribution remains largely unaffected if smaller amounts are used. In contrast, usage of TEB resulted in only small amounts of SCB while the MWD was broadened, which was related to increased early-stage PE densities.
Additionally, our results have also shown that the densities of these early-stage PE materials is lower than what is expected for bulk counterparts. This was attributed to the fact that the dimensions of the PE crystallites were similar to the size dimensions of the pore network of the catalyst, which hereby regulated the crystallization and related density to a significant extent.

Bio-based rheology modifiers for coatings – Delft University (CHEMIE.PGT.2017.009)
Organic rheology modifiers for solvent based coatings are superior to inorganic rheology modifiers with respect to coating production, application and appearance, and moreover, they have the advantage that they are biodegradable and can be produced from renewable resources. These organic rheology modifiers are made by a self-assembly process of organic molecules into organic fibrous dispersions, which involves the lengthy and energy-consuming thermal annealing of semi-crystalline powder into crystalline fibers, requiring narrow process conditions. This tedious fabrication process under stringent conditions severely limits adaptation to specific applications and customer requests, and also enforce centralized production of the fibrous dispersions to guarantee product quality.

In this project we have been able to develop a faster, more robust, and more flexible production process, which will lead to significant reduction of energy usage. Moreover, the new production process allows a much better control of the product quality which will lead to a significant reduction of waste. As a spin-off to

this project we have developed a new data processing method for calorimetric analysis methods, which will make this widely use analytical tool more versatile for especially formulation technology.

Innovation by Product and Process Design: For life sciences & health, energy conversion & storage, circular economy – Delft University (CHEMIE.PGT.2017.010)
The aim of the TKI program "Innovation by product & process design" for the TU Delft post-MSc PDEng programs in (bio)chemical engineering design is to strengthen the product and process design competencies and intensify the cooperation with industrial partners in the following fields:
• Life sciences & health
• Energy conversion & storage
• Circular economy
and seek intensified cooperation with companies active in the research, discovery and design of products (and their manufacturing processes). PDEng Individual Design Projects can be a very efficient catalyst for initiating the aimed cooperation and to arrive at novel products and processes.

In the TKI program and according to the design of the program we have been able to successfully:
• Identify possible industrial partners with (core) activities in the fields of circular economy (4 projects) and energy conversion & storage (1 project). These 5 projects were executed in the period 1 January 2018 to 31 January 2020. Companies involved in these projects were: ConXys International Technology B.V., IHC MTI B.V. part of Royal IHC, Proton Ventures B.V. SLOOP Consulting B.V.
• Formulate design projects that were novel, innovative developments in which the design focussed on the best design options and recommendations to further improve the product/process for a sustainable application.
• Devise innovative designs that pave the ground for further development towards implementation.

The companies involved in these projects were: Conxys Technologies International B.V.,
The execution of these 5 projects made it clear that the design methodology and approach developed at TU Delft and applied in PDEng projects in other fields (oil & gas, bulk and specialty chemicals) were also well applicable in these projects and have delivered novel design solutions for flexible packaging design and recycling, for in-situ COAX3 cable replacement by Hybrid Flexible Fiber, scale-up of the Battolyser technology, and geopolymer binder production.

Rheology and microstructure of concentrated polymer blends with viscoelastic components – Eindhoven University (CHEMIE.PGT.2017.013)
The rheology of the blend components can include several complexities such as normal stresses in shear, shear thinning and strain hardening in extension. To allow to pinpoint the contributions of the different above-mentioned factors, a systematic study will be performed in which as much as possible different contributions are isolated. This will be essential to generate the required information for the development of a framework that is generally applicable and system and process independent.

For the design of the setup and experimental approach, three main aspects were considered namely the optical setup for the interferometry experiments, the contact cell that needs to be placed in this optical setup and that allows to generate film drainage and the materials chosen for the research. For the optical setup, the main design consideration is the use of white versus coherent light. Whereas the former option simplifies the data analysis procedure especially for non-monotonic evolutions of the film thickness, the latter option allows to characterize larger film thicknesses and up to larger speeds. Hence, the latter option was chosen. Moreover, as compared to similar setups available in literature, the optical train is modified to allow for the use of a second reference wavelength, which results in absolute rather than relative thickness values, and the laser light is focused on the film to allow for enhanced signal-to-noise ratios. This results in a versatile optical setup suitable to study film drainage between two polymeric materials that in general

have limited contrast in refractive index (see figure 1). A sample cell is designed that allows droplet approach to occur both with a constant force through sedimentation as well as with a controlled speed by moving a needle with a pendant droplet (see figure 2). This allows to investigate different situations relevant for actual processes in which the contact force and speed vary during the approach of two droplets. Finally, based on an analysis of the flow fields between two approaching droplets and a literature survey on the rheological parameters of different fluids, an estimate was made of the expected viscoelastic stresses and required droplet dimensions to ensure the presence of viscoelastic effects during the experiments. Moreover, chosen materials should be immiscible, have a significant contrast in refractive index and density, should not contain interfacially active components and allow for variation of the elastic properties. Based on this analysis, a specific type of Boger fluids, based on polyethylene oxide in water were selected as the matrix phase whereas polydimethylsiloxane was selected as the droplet phase. Drainage experiments showed that there was a clear effect of the PEO on the drainage process of the droplets, which hints to effects of the viscoelastic matrix on the film drainage. However, there may be some effects of PEO going towards the water-PDMS interface that contribute as well. Therefore, additional experiments on another blend system are required to finalize a full dataset that allows clear interpretation of the phenomena.

Scalable synthesis of hig-efficiency organic dyes for colourful building integrated photovoltaics – UvA (CHEMIE.PGT.2017.014)

This project explored scalable routes to porphyrin-based dyes for application into inkjet printed, dye-sensitized solar cells (DSSCs). DSSCs are unique in that they do not require expensive cleanroom facilities for fabrication while exhibiting superior low/diffuse light power conversion efficiency (PCE), making them perfect for application in the Netherlands. The 1st generation of this technology relied on ruthenium-based dyes, which exhibit weak color, i.e. more dye is needed to absorb all available sunlight. Dyes based on porphyrins demonstrate stronger absorption coupled with higher PCE, doing more with less while removing the use of the rare element ruthenium. Porphyrin-type dyes are related to naturally occurring chlorophyll in green plants, which has a vibrant color and is used by nature to absorb light and power photosynthesis. The availability of a scalable, high-efficiency green dye bolsters the application of DSSCs to building integrated photovoltaics (BIPV), where aesthetic design features such as patterning, color and transparency play a greater role in technology adoption than typical rooftop solar installations. This project improved the sustainability of key porphyrin building blocks by dramatically reducing the amount of waste (solvent, silica) generated in a scalable synthetic procedure without any chromatography. Furthermore, a proof-of-principle was achieved for a chromatography-free synthesis f the porphyrin sensitizer LD14-C8 (pictured). With these two components coupled together, the possibility of a scalable and sustainable synthesis of porphyrin dyes can be realized. The final porphyrin dye was implemented into transparent, colorful solar modules by inkjet printing, demonstrating that dyes with vibrant color can be applied to improve the suitability of DSSC technology for BIPV applications.

NWO Programmatoeslag 2016; deelprojecten NWO LIFT ´The impact of novel modulators on the fate of (mutant) Cystic Fibrosis Transmembrane conductance Regulator (CFTR), 2) Chemical Ecology Based Screening Platform for Novel Growth Modulators From Actinomycetes (ChemoScreen); 3) Antisense oligonucleotide therapy, a novel molecular approach to restore CFTR biosynthesis in cystic fibrosis patients – NWO (CHEMIE.PGT.2017.015)

Present day treatment of CF requires a combination of at least 1 'corrector' to increase the amount of CFTR on the plasma membrane and to open those molecules with a so called 'potentiator'. Galapagos/AbbVie developed new medicines for Cystic Fibrosis (CF). The aim of this project is to assess how the new compounds of Galapagos/AbbVie increase the amount of cellular CFTR. This could either occur through improvemed folding of newly synthesized CFTR molecules but also by reducing the disappearance of CFTR from the cell surface by endocytosis. The methods we developed can measure the effect of both the indivual as well as of the combined compounds. The Galapagos/AbbVie potentiator was first thought to have a istinct

mode of action than VX-770 of Vertex Pharmaceuticals. We however discovered when taking differences in affinity into account that the Galapagos/AbbVie potentiator acts according to the same principle as VX-770. The C1 and C2a correctors act synergistally on F508del CFTR, where C2a activity is enhanced by the presence of C1. C2a also can improve other CF-causing mutants and likely acts to 'freeze' the protein which causes it to become less sensitive to degradation effectively 'stabilizing' CFTR on the cell surface. We also discovered the domains in CFTR that the correctors act upon. Although C1 only acts on TMD1, this does not hold for C2a. In this project we developed a unique and versatile toolbox of assays and reagents to analyze folding of CFTR. The toolbox is now used extensively in a multitude of projects in the Braakman-vander Sluijs group. Our toolbox may also lead to new collaborations with industrial partners to dermine the mode of action of coumpunds on CF or other mono-genetic diseases.

731.017.409; In dit onderzoeksproject hebben we als doel om een nieuwe pijplijn op te zetten voor het testen van Actinomyceten uit de collectie van Universiteit Leiden voor de productie van bioactieve stoffen die de groei van zoogdiercellen kunnen beïnvloeden. Voor dit project is allereerst een nieuw cultivatie systeem ontworpen waarbij de bacteriën groeien op vast agar medium gescheiden door een semi-permeabele membraan van de zoogdiercellen. Dit nieuwe cultivatie systeem laat directe diffusie van actieve stoffen toe over de membraan in beide richtingen. Van dit nieuwe systeem is een prototype gemaakt, getest en geoptimaliseerd. Daarnaast zijn de juiste condities gevonden van groeimedium van de bacteriën en de zoogdiercellen, zodat deze gezamenlijk te groeien zijn in het cultivatiesysteem.

731.017.420:
In CF patients, the salt-water transport is disrupted, causing the mucus in the lungs to become tough (cystic fibrosis). The cause of this hereditary condition is an error in the DNA, which is passed on in the mRNA, which is translated into a defective CFTR protein. In contrast to the
current CF drugs that act on the protein level, there is now a drug under development that acts on the mRNA level. By investigating how manipulations of the mRNA and its translation affect CFTR structure and function, we will understand how this new drug works, which is needed to accelerate its development and improve it over time. Over the past year, research has focused on understanding how the mRNA can influence the structure and function of CFTR. A number of different, so-called 'silent' mutations have been investigated for this, in which the mRNA code is changed, but in which these changes do not affect the building blocks (order) of the protein chain read. Changes in structure and function are then only caused by changes in eg speed of the reading process. All the mutations examined caused differences in the production of CFTR, even though the codes of only 3 to 5 ""letters"" (out of 1480) were changed.

Smart design of emergency relief systems – Eindhoven University (CHEMIE.PGT.2017.016)
Safe storage of chemical compounds is not trivial, since these are often mixtures that contain various components that produce heat upon reacting and are compressible. If a sudden breach in a vent system occurs, or in the safety valve applied, the mixture swells by flashing, the generation of vapor bubbles can occur, in particular in the throat, the place with the smallest cross-section. Conventional design methods gave safety valve cross-sections in the order of the diameter of the storage vessel. The novel design method is validated and yields practical values for diameters of vent system and safety valves.

Development of electrochemical cleaning of washing water flue gases – ECN (part of TNO)
(CHEMIE.PGT.2017.018)
Recovery of hydrochloric acid from flue gas; the next step from waste incineration to raw material factory
As part of the wet-chemical cleaning of flue gases, flue gases released during the incineration of waste are passed through a scrubber. Acidic components are washed out of the flue gases, and the acidic washing water is neutralized with strongly alkaline raw materials. The residue formed in this process consists of a filter cake that mainly consists of gypsum and that is heavily contaminated with metals and other contaminants. This filter cake is dumped in the Netherlands. The remaining treated water contains a lot of salt and should not be discharged.

Aromatics from shrimp shells – Groningen University (CHEMIE.PGT.2018.003)
This project aimed to use the increasing amount of shrimp shell waste streams in the Netherlands for the production of valuable chemicals. One of the main components of shrimp shells is the natural polymer chitin, which can be utilized to synthesize plastics or pharmaceutical drugs with new properties. To do this, chitin can be modified in various ways. In this project, a combination of mechanical and chemical modification was chosen to access precursors from chitin which are not commercially available. These precursors were subsequently reacted to probe the possibility for converting these to chemical building blocks. New compounds with interesting properties were synthesized. These compounds along with the knowledge gained in this project provide a basis for further research towards commercial products directly from waste streams high in chitin.

Development of Continuous Bio-Aromatics Process FIAD2 (Crossover with TKI Agri&Food) – TNO (CHEMIE.PGT.2018.014)
The FIAD 2.0 (Furanic Intermediates and Aromatic Derivatives) project has now been completed. An important part of the project was the collaboration with industrial end-users evaluating the application potential of such compounds. In Phase 1, 3kg of bio-based HMA was prepared and this was tested in lubricant and polyurethane applications. Based on feedback on the samples from industrial partners, the production protocol was adapted to produce a further 10kg of HMA with an improved product specification for further application testing at the industrial partners. The HMA-based products which were prepared from these materials have been shown to have promising properties. On top of the sample production, two of the three process steps for the production of HMA have been transferred to, and validated in, scalable continuous flow reactors, laying the basis for further scale up. The technoeconomic model has also been further refined.

BPM programme (FOAMEX-II + DISCOVER-II) – Wageningen Food & Biobased Research (CHEMIE.PGT.2018.016)
FOAMEX-II: Advances in foam extrusion of PLA:
Poly (lactic acid) PLA is one of the most attractive biopolymers. It combines a low ecological footprint with good material properties and biodegradability. Moreover, PLA is one of the most affordable biopolymers. Nowadays PLA can be processed via several techniques including film casting, injection moulding and thermoforming making it applicable in several products in the market. However, some inherent properties of PLA have limited its use in commercial extrusion foaming. Within the FOAMEX-II project, the participants have taken the production of PLA based extrusion foams to a next level where its applicability in foamed products has become possible. For a commercial breakthrough, improvements were still needed with respect to rheology and crystallinity of the proposed formulations and materials. In the project, formulations and (more important) concepts were optimized in order to make them even more commercially interesting. The optimization of the materials focused on the requirements of the market, i.e. a broad and stable process window, sufficient crystallinity, melt strength and an interesting cost price.

DISCOVER-II: Development of an innovative, sustainable roofing system:
The DISCOVER-II project aimed at the development of a biobased alternative to conventional roofing membranes, such as bituminous or synthetic roofing. In this project, Wageningen Food & Biobased Research worked together with roofing producer BMI (formerly Icopal) and Stora Enso.
Conventional flat roof covering systems such as bitumen or synthetic polymer based membranes are of high quality and have a long service life, however, they are mainly made from petroleum resource. Since this fossil resource is finite and its extraction, refining and use contributes to climate change, there are ample reasons to consider more sustainable alternative materials while retaining the required technical and functional characteristics of roofing membranes.

Biobased roofing:
The ultimate goal of the project was the development of an environmentally friendly alternative to bituminous roofing systems, in which the fossil bitumen has been replaced by biobased raw materials. In the DISCOVER-II project a large range of biobased streams was evaluated. One important issue is that biomass

derived streams are less hydrophobic and more reactive than bitumen. Focus was given to side streams which are available in large quantities from the pulp&paper and agri&food industries.

Results on the evaluation:
Binder mixes were designed based on fully biobased components comprising for example lignin and vegetable oils. These binders were manufactured at lab scale up to around 1kg and evaluated for its main characteristics such as mixing ability, homogeneity, visco-elastic and rheological behavior, penetration value and stability. The results are close to the desired range of properties for sustainable roofing systems. Industrial applicability with current manufacturing principles seems possible with these innovative materials. LCA results indicate that the use of biobased streams can have a significant benefit, giving a lower carbon footprint, especially if the biogenic carbon sink function is taken into account.

Towards high-current density electroconversion processes – Delft University (CHEMIE.PGT.2019.001)
Electrolysis is a chemical process where electricity can be used to turn one molecule into another. The electrolysis of water, CO2, and nitrogen-based compounds are all options to turn waste gases and compounds into valuable compounds. Such a technological option may allow for the usage of fossil fuels to be reduced by creating useful products in a greener way.

Electrolysis devices, however, are complex in nature. Scientists and engineers then use several key metrics (e.g. efficiency, selectivity, reaction rate and stability) as a means of judging how well or poorly an electrolysis device operates. We can then find ways to improve these metrics, which makes the technology a more viable economical option versus current fossil fuel-based technologies.

In this project, we use infrared radiation as a means of visualizing the performance of electrolysis devices. This approach then provides more information than traditional ways of analysing these systems. report the usage of infrared thermography to map the electrochemical activity of a gas-diffusion electrode performing water and CO2 reduction. By associating the heat map to catalytic activity, the presented system can capture electrochemical and physical phenomena as they occur in electrolyzers for large-scale energy applications. We demonstrate applications for catalyst screening, catalyst-degradation measurements, and spatial activity mapping for water and CO2 electrolysis at current densities up to 0.2 A cm−2. At these current densities we report catalyst temperature increases (>10 K for 0.2 A cm−2) not apparent otherwise. Furthermore, substantial localized current density fluctuations are present. These observations challenge assumed local conditions, providing new fundamental and applied perspectives.

Reosim – Eindhoven University (CHEMIE.PGT.2019.003)
Plenty of soft materials all around us consist of drops or bubbles of one fluid distributed in another fluid. These fluids do not mix, unlike sugar or salt that do dissolve in water. For example, when you try to mix oil and water, after leaving the fluid at rest you will see that the oil floats to the surface and forms a layer on top of the water. Oil and water are said to be immiscible. The chemical and mechanical properties of immiscible fluids are taken advantage from in a lot of applications varying from everyday consumer care products and foods to pharmaceuticals, petrochemicals, and polymer blends. The presence of an interfacial layer in between the immiscible fluids yields a completely different structure on very small length scales in the mixture than in the constituent fluids separately. The holy grail is synergy of properties: the mixture has more beneficial/desired properties and performance than the fluids separately.

The goal of this project is to study the flow behaviour of immiscible fluids using computer simulations. By varying the mechanical properties of the interface in between a single drop suspended in another fluid, we gain insight into the influence of the interface on the flow of the mixture. This enables to predict and control final properties and performance of products by providing design rules in material choice and processing. For this purpose, a computational modelling framework has been developed which has been shown to describe the stress-strain behaviour of interfaces as observed in the literature. Conclusions so far: by including elasticity to the interface, meaning that it can store more and more energy upon deformation, you need to apply a stronger flow to deform the drop.

Towards the Biomass Genome – Utrecht University (CHEMIE.PGT.2019.019)

Global energy usage and anthropogenic greenhouse gas emissions have been increasing ceaselessly during the past few decades. Due to the inevitable consequences that arise from climate change, there is an urgent need to find a sustainable alternative to fossil fuels. An important alternative to fossil fuels is biomass, which can be converted into sustainable fuels and chemical building blocks via catalysis. The composition of biomass and biomass-derived fuels is typically rather complex and strongly depends on the actual input substance that is used. For example, the bark of an oak tree will have a different chemical structure compared to a shrimp shell and will consequently suit a different application. To make biomass-derived fuels a viable alternative, it is important to understand how a certain input feedstock leads to a certain fuel composition. To aid this process, we established an electronic database for biomass-related compounds. The database provides a platform for researchers in the field to share and access relevant data, promoting openness and collaborations amongst research groups.