

Projects with PPP programme allowance 2017

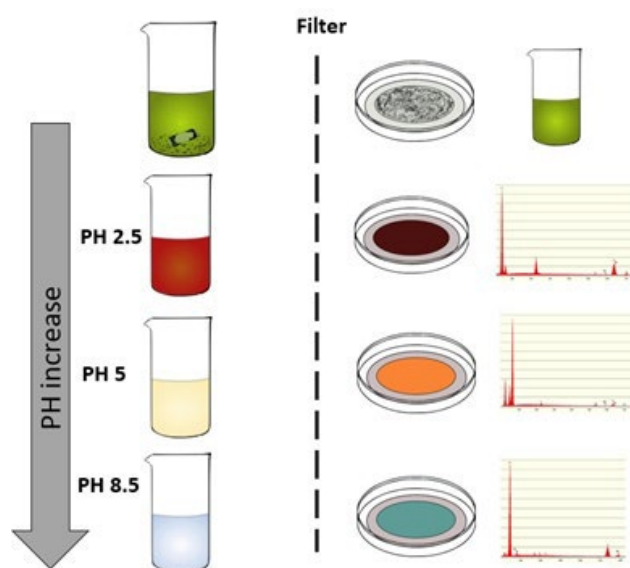
Closing the loop of the Electrochemical Machining Process – RUG

(CHEMIE.PGT.2018.004)

In this research, we tackled the pressing issue of our ever-increasing global demand for metals. We found a way to recover valuable metals from a solution used in a manufacturing process, like recycling gold from old electronics. This process allowed us to separate these metals into different types, like sorting different coins.

We faced a challenge because the solution also contained various types of metals, making it a bit like sorting a mixed bag of coins. We decided that using a method called leaching was the most practical way to separate these metals. Other methods, like using special filters or magnets, were too expensive and complex for this task.

The sludge we worked with contained not just metals but also other things like salt and nitrate, which we found ways to recycle too. We even discovered a method to recover sodium nitrate, which is useful for making batteries, like recharging your phone.



This research was successful in finding ways to recycle valuable metals and other materials, making our metal use more sustainable and eco-friendly. It's like turning old coins and metal scraps into shiny new ones while also helping the environment. The market analysis showed that the current sludge's metal value isn't high enough for profitable recycling, covering just the separation costs. Yet, as the push for eco-friendly practices grows, future separation could become profitable. Many industries, like aerospace and textiles, face similar waste issues, sparking interest in sustainable solutions.

Stofoverdracht in waterelektrolyse – TUE

(CHEMIE.PGT.2018.005)

Production of green hydrogen is one of the cornerstones for making the chemical industries sustainable. A mature technique for producing green hydrogen is alkaline water electrolysis. In this process green electricity is converted into small hydrogen bubbles that are produced on the electrode surface. The presence and transport of these bubbles affect the efficiency of the electrolysis process. In this project numerical simulations were carried out to characterize the bubble transport for a well defined testcase. A robust set of simulation sub-models and settings was obtained that can be used to carry out predictive simulations of electrolyzers of different geometry. In future research the simulation tool can be used to de-bottleneck and optimize electrolyzers.

Drying of colloid-polymer mixtures and the role of interactions and phase stability – TUE

(CHEMIE.PGT.2018.006)

Colloidal mixtures and block copolymers are abundant in soft matter. For certain compositions, these types of systems tend to (micro-)phase separate and demix into coexisting phases that differ in composition, structure,

and properties. In this project, theoretical models were developed that allow to predict how certain parameters affect such phase transitions which can be used to guide experimental work. The results can contribute towards the design of stable soft matter systems with desired properties for their applications in coatings, pharmaceuticals and food, and provide significant insights into phase transitions of natural colloidal systems like clay, blood and living cells.

During this project, theoretical concepts originally developed to study phase behaviour of colloid/polymer mixtures were improved, which can now be applied to colloidal mixtures. The stability regions of different types of (coexisting) phases for colloidal mixtures were investigated for a wide range of size ratios, shape parameters, and concentrations. The model predictions are in close agreement with experiments and computer simulations performed by collaborators. The theory also revealed a variety of interesting phenomena such as the possibility of demixing into five different coexisting phases in a dispersion containing only two colloidal components. Moreover, the phase behaviour of block copolymers was investigated using self-consistent field theory. Block copolymers can spontaneously order into macroscopic phases with periodic domains in the nanometer scale. It was shown how solvents can be used to manipulate the size and shape of these domains which is of interest to fabricate block copolymer materials with specific optical or electronic properties. It was also shown how the surface affinity of block copolymer surface modifiers in coating formulations is affected by drying. The results supported experimental findings, which revealed that the distribution of block copolymers over bulk and surface can significantly deviate between wet coating formulations and cured coatings.

Alkanes Conversion: Design, Characterization and Performance of Bifunctional Catalysts – UU

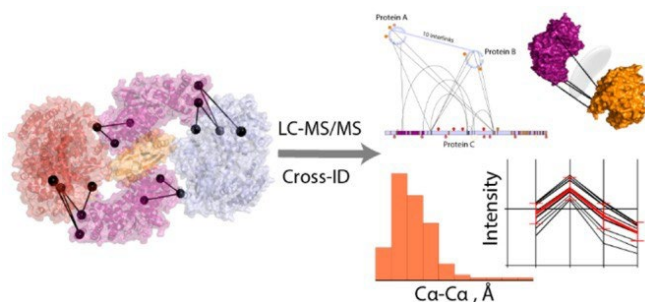
(CHEMIE.PGT.2018.007)

Maximizing the utilization of noble metal atoms by manipulating the metal dispersion, metal-support interaction and location is critical for heterogeneous catalysts. In this project, we explore the low limit of platinum usage in hydroconversion of n-alkanes for the industrially relevant bifunctional catalysts consisting of platinum, zeolite and alumina binder. A series of composite catalysts with different loadings of platinum selectively deposited on alumina binder, on zeolite crystals or inside zeolite crystals have been prepared. We demonstrate that by rational organization of functional sites in nanoscale, the usage of platinum in bifunctional catalysts can be reduced by more than an order of magnitude from 0.2 wt% to 0.01 wt%. The catalytic activity has not to be compromised, while the isomer selectivity is even enhanced by placing trace of platinum nanoparticles on alumina binder or on zeolite crystals. In contrast the catalysts with platinum inside the zeolite crystals, often derived from the conventional ion-exchange or impregnation methods, exhibits inferior isomer selectivity and catalytic stability. A general criterion has been proposed for decreasing the usage of platinum source by rational spatial organization of different functional sites.

Combining crosslinking mass spectrometry and structural modelling to interrogate the architecture of Tau interaction networks within neuronal cells – UU

(CHEMIE.PGT.2018.008)

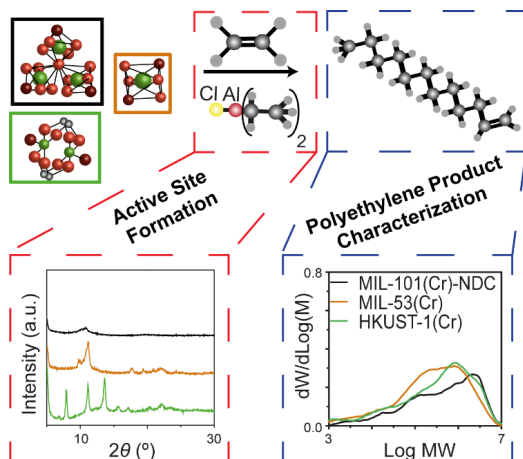
You have soul mates who are always near each other and passersby who just happen to hook up – plus everything in between. Often we need to hook up to make things work. That's how the social structure of human society works, but that's how it works with proteins in the cell. Proteins are involved in all natural processes in our cells. We know that a human cell contains at least 20,000 different proteins, but we only really understand how a cell works if we know which proteins work together, and how they do this. In this project we used chemical handcuffs ("cross-link molecules") to discover which proteins are close to each other at any given moment in the cell. Because the crosslink molecules have a fixed length, we know which amino acids are close together. We used mass spectrometry to identify exactly where the handcuffs are attached to the proteins, and thus we were able to visualize which proteins are "active" in a certain process and which additional proteins are "guilty by proximity". This helps us to understand better how biology and life happens at the molecular level.



Scheme of Cross-ID used to detect and visualize protein-protein interactions in the cell

New Insights in the working principles of tri-ethyl boron as co-catalyst in Cr/SiO₂ Phillips catalysis – UU (CHEMIE.PGT.2018.009)

In the Scanning Transmission X-ray microscopy (STXM) related work we found that the polyethylene (PE) density can be tailored by selecting the proper type and amount of co-catalyst. The early-stage PE materials produced with tri-ethyl borane (TEB) demonstrated larger densities than those produced with tri-ethyl aluminum (TEAL). This difference was ascribed to the enhanced degree of Short Chain Branching (SCB) with TEAL while the Molecular Weight Distribution (MWD) did not increase much. In contrast, usage of TEB resulted in relatively small amounts of SCB while the MWD was broadened, resulting in materials with larger densities. Secondly, STXM also revealed that the densities of these early-stage PEs was lower than what expected on basis of their bulk properties, attributed to the fact that the PE crystallites are in the size dimensions of the pore network. Which hereby restricts free crystallization resulting in the related lower PE densities.



The second part included investigating the viability of Cr-based MOFs as ethylene polymerization catalysts. In our research we found that one of the major prerequisites for ethylene polymerization is the ability of the MOF to be activated by the co-catalyst, this activation was related to some degree of leaching: with a maximum of 5% of the Cr content leaching into solution. Spectroscopic investigations into this activation procedure as well as analysis of the PE materials have revealed that the MOFs cannot be considered heterogenized single-site catalysts after activation with the co-catalyst. In conclusion, we found that MOFs can be exploited as ethylene polymerization catalysts, with the prerequisite of “activation” being established in this work.

HiBriDLight: High Brightness Diode Pumped Light Concentrators – UU (CHEMIE.PGT.2018.010)

In the field of lighting there is a great benefit in moving from conventional technologies as well as laser light sources to LED-based light sources to overcome environmental, safety, lifetime, performance issues and to reduce cost. Due to the limited brightness of conventional LEDs as compared to e.g. discharge lamps, many high brightness applications at the moment still cannot be realized with LED-based solutions. Although LED brightness is still increasing, the requirements of many high brightness applications are far higher than what can be achieved with the expected evolution of LEDs.

To realize scalable high brightness light sources, recently optical systems consisting of multiple blue LEDs pumping a luminescent concentrator (see Fout! Verwijzingsbron niet gevonden.) have been developed. The central light conversion module is a convertor rod, which can be a ceramic Ce-doped garnet rod. State-of-the-art systems relying on this technology (e.g. ColorSpark HLD LED technology) however still show significant intrinsic light losses, especially at high pump powers.

This project aimed at reducing efficiency losses at high pump powers (‘droop’) by providing insight in loss processes and relating these to material properties optical processes with the ultimate goal to realize highly

transparent luminescent concentrators with improved brightness. The project has provided clear evidence for droop by excited state absorption and reduced droop for LuAG:Ce concentrator rods annealed in air. Air annealing oxidizes part of the Ce³⁺ to Ce⁴⁺. Quantitative analysis shows that through air annealing the droop can be reduced by a factor of ≈ 3 . These new insights are important for the development of optimized concentrator rods with reduced droop and, at the same time, provide insight in the limitations of output power related to droop that cannot be avoided.

Industrieel Hergebruik van End of Life thermoharde composieten – WHS

(CHEMIE.PGT.2018.011)

Wind Energy has become part of daily life and thermoset composite materials are crucial in the construction of these giant wind mill blades: blades of the current large size can only economically be produced from thermoset composite materials. However, up till now these kind of materials were non-recyclable because they can not be recycled in the classical way – separating them into their base components is not possible without losing their value. The European approved recycling route for these thermoset composites involves retrieving the calorific value using cement kilns – effectively, you burn it and get heat back in return.

A different solution needed to be found, one that brings value based on the strong characteristics of the old material, instead of the value destruction that comes with burning. Together with a large industrial consortium



the Windesheim Professorship for Polymer Engineering came up with a way to reuse these old wind mill blades (or yachts, or train parts) by using them as a reinforcement material for new composite parts: Reuse of End-of-Life Composite Materials.

An industrial and economically sound route was found to produce new composite based on flakes and strips of old yachts and windmill blades. Demonstrators like crane mats, furniture, retainer walls, support beams and berthing structures were produced, placed at various locations in the Netherlands and are currently being monitored for their performance.

3DPrintHuge – PSP

(CHEMIE.PGT.2018.012)

The goal of this research is to investigate the large-scale industrial 3D printing of recycled thermoplastics. A test set-up was realised to study 3D printing of polypropylene recycled. Cylindrical test objects up to 60 cm in diameter were produced. This created a lot of knowledge about how to steer in the printing process and how to obtain an object with good mechanical properties. Printing with semi-crystalline material is complex and requires precise process settings with a small processing window. It also requires good knowledge of the material. During this research, we learned a lot about the material and the influence of the process parameters. With this knowledge, the further development of large-scale 3D printing of semi-crystalline plastics can be further exploited.

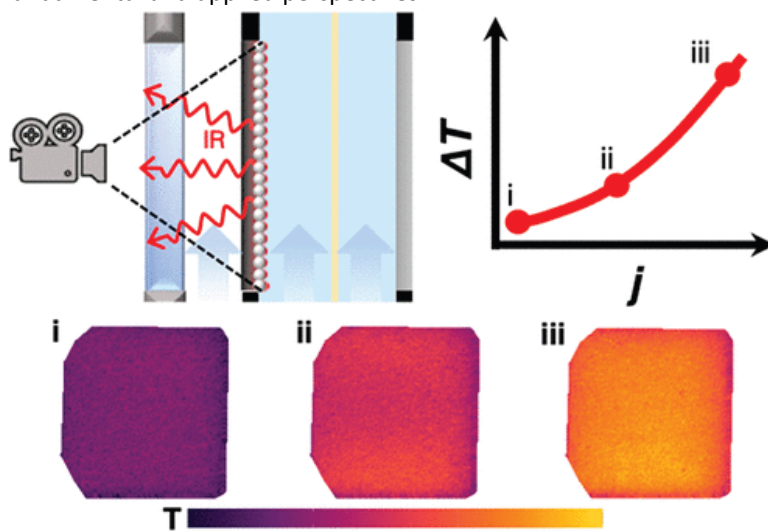
TT1 – High current density electrochemical processes – TUD

(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 gasdiffusion 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.



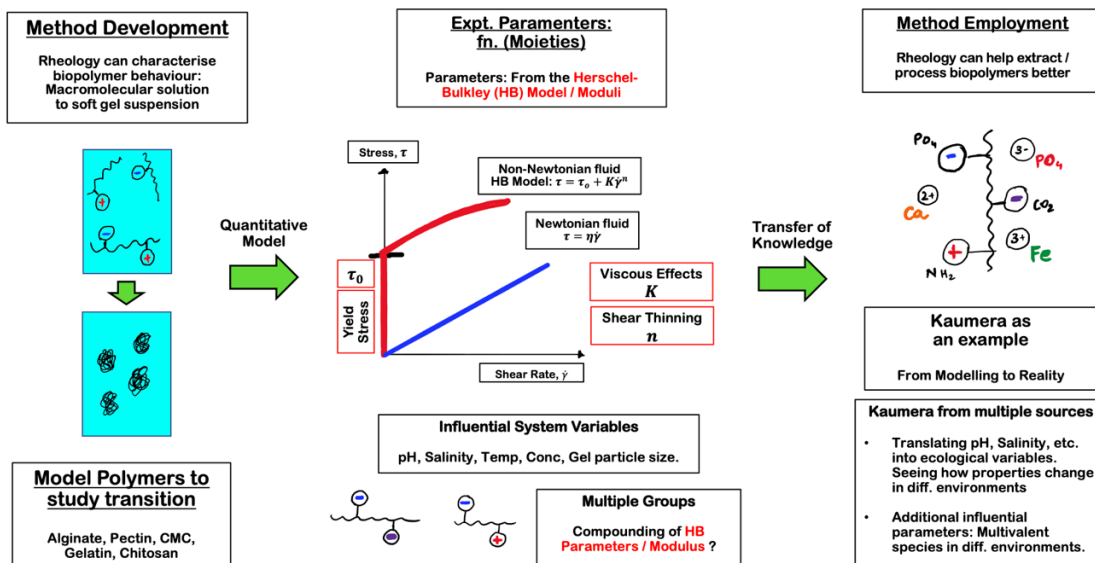
Van afval naar grondstof: Kaumera/ Production and Characterisation of Kaumera – TUD (CHEMIE.PGT.2019.014)

Kaumera is a potential high-quality biopolymer that is extracted from wastewater streams. Initial studies have revealed that Kaumera is representative of a valuable wastewater biopolymer that can have applications in the building and construction industries. However, as a glycoprotein, the chemical characterisation of biopolymers such as Kaumera remains elusive. This comes down to the fact that a hundred and twenty potential monomer units could combine in different combinations to form the structure of the Kaumera biopolymer.

The current research is geared towards overcoming this problem by understanding the charged functional groups on the biopolymer and assessing how they impart functionality. Techniques such as gel electrophoresis has revealed the different types of charges that can exist within Kaumera. This, along with techniques such as infrared spectroscopy has revealed that Kaumera can also be used for applications demanding flame retardancy. Additionally, techniques such as rheology aims to map the influence of these groups on the mechanics of the biopolymer. So far, rheology measurements conducted with other biopolymers reveals that there may be a persistence of generic trends for all biopolymers. This helps establishing a systematic investigation technique for unknown biopolymers such as Kaumera under a variety of conditions. This can further help in identifying how the source of extraction / protocol for extraction impacts the final mechanical properties of the polymer.

The holistic outcome from the current research is a deeper understanding of Kaumera's functionality and a further broadening in the applicability of wastewater biopolymers.

The Rheo-Chemical Characteristics of Biopolymers



Hypothetical Conference styled Poster outlining the approach adopted by Anand Raja (ChemE) over the course of his PhD. Flowchart provides an insight into how gelling in biopolymers can be translated

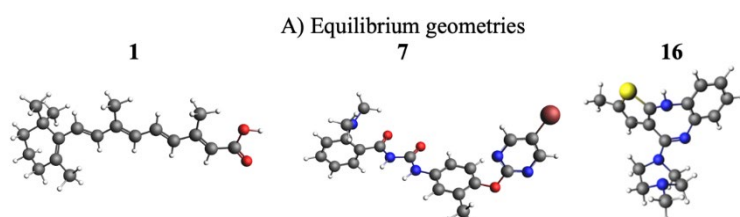
Better and faster conformer generation for different types of molecules – UvA

(CHEMIE.PGT.2019.017)

Molecules in the gas phase or in solution are continuously moving, vibrating, and switching between different structural conformations, or conformers. Larger molecules typically have more conformers and the number of conformers that a molecule can adopt at a given temperature depends on the energy distribution of these conformational microstates and the energy barriers that separates them from each other. The ensemble of accessible conformers underlies all sorts of material properties, including spectroscopic response, crystallization behaviour, polymorphism, solvability, and reactivity.

Exploring the conformer space with quantum chemical modelling methods is a daunting task for all but the smallest molecules, which hinders the interpretation and prediction of experimental observations, such as UV/Vis and CD spectra, and design of compounds and materials, such as protein inhibitors, optimal catalysts, and the crystal packings of pharmaceuticals, to name but a few.

In this project we used the metadynamics (MTD) algorithm to explore the conformational space and the chemical reaction space of a library of organic molecules, a promising approach recently introduced by Grimme in combination with the semi-empirical modeling. MTD enhances the sampling of the configurational space by gradually constructing a repulsive bias potential onto one or more order parameters, to escape free energy minima and overcome free energy barriers. We will use the root mean square deviation (RMSD) as the CV to drive molecules away from an initial (meta-) stable conformer state to find new conformers. MTD, as implemented in the Plumed software, has recently become available within the ADF software suite, which give us access to a variety of levels of theory to describe the atomic interactions. This allows for example for dealing with large molecular systems and for exploring reactive pathways in a simulated nanoreactor.



Spatiotemporal operando studies of automotive catalytic reactor – TUD

(CHEMIE.PGT.2019.018)

The design of catalysts and functional materials in modern devices is largely dependent on empirical trial-and-error approach. Useful empirical relationships between catalyst material and performance may be possibly established; however, this approach needs a large amount of time and manpower to reach desired performance, and for this reason the current functional devices are often the results of serendipity and intensive optimization of extensive experimental parameters. Once an empirical material structure vs. performance relationship is established, rational design of functional devices can be in principle facilitated.

However, this is not fully true as represented by the case of automotive catalytic converters where large gradients of material structures, oxidation states, concentrations (gas phase and surface/bulk species) and temperature exist as a consequence of chemical conversions processes. Even worse, in practice the gradients fluctuate and vary with time within the catalytic converter.

Reflecting the background, this project identified the nature of active surface chemical species, surface/bulk structures of catalyst, gas phase species, temperature and their spatial gradients within catalytic reactors of high relevance for the automotive industry. The state-of-the-art spatiotemporal analytical tools such as gas sampling and temperature detection were developed to enhance the quality and complementarity of physicochemical information within catalytic reactors. Through the information, the mechanistic details and support effects of CO oxidation over Pt were elucidated. Furthermore, the gained information was used as an input for simplified yet practical kinetic modelling of catalytic processes to extract intrinsic kinetic parameters to precisely express chemical reactivity and redox properties of catalyst materials on the reactor scale.

Unravelling Fabry disease: establishing toxicity of lysoGb3 and identifying additional toxic storage compounds – LEI

(CHEMIE.PGT.2021.005)

Fabry disease is a common lysosomal storage disease due an inherited defect in the lysosomal α -galactosidase A (GLA). Consequently, Gb3 and lysoGb3 accumulate. There are indications for additional, yet unknown, substrates of GLA, that accumulate in Fabry patients and contribute to symptoms. Our research on zebrafish, that normally lack Gb3 due to absence of the synthetic enzyme A4GalT, provides concrete evidence for this. Fabry fish lacking GLA as well as lacking Gb3 and lysoGb3 develop nevertheless kidney pathology. The animals offer an excellent source for the identification of the additional GLA substrate. In addition zebrafish should allow us to examine whether presence of lysoGb3 contributes to severity of Fabry symptoms.

Technology Areas Polyolefins en Coatings technology - DPI

(CHEMIE.PGT.2018.001)

#802 "Structure determination at the nanoscale and atomic dynamics of $MgCl_2$ primary particles in Ziegler-Natta catalysts"

Research on Ziegler-Natta (ZN) catalysis is projected to understand the ensemble structure and the interplay among $TiCl_4$, donors, $MgCl_2$ and the Al-activator. Even though a certain progress has been made on the local structure of the active Ti sites, the knowledge of the identity of δ - $MgCl_2$ was still quite limited. In this project, JAIST and UNITO teams revisit the structure and morphology of δ - $MgCl_2$ as the primary particles of ZN catalysts by experimental and computational techniques, including machine-learning-aided modeling, X-ray scattering, and vibrational spectroscopies.

#803 "HEat Management in Polymerization Reactors (HEMPR)"

To study the effects of liquid injection on the bulk behaviour of the bed, fluidization experiments were performed in a pseudo-2D fluidised bed. Firstly, the measured particle temperature distribution was used to quantify the the temperature uniformity in the bed without liquid injection. For several fluidisation regimes, the degree of temperature non-uniformity was quantified using Infra-Red Thermography (IRT). The particle temperature distributions were obtained from the whole-field temperature data, which were characterised using the standard deviation, i.e. the width of the distribution, and skewness, i.e. the dominant temperatures in the distribution.

Based on the heat loss data and bubble frequencies, the standard deviation and skewness revealed to be good indicators of the temperature uniformity for the studied fluidisation regimes.

Subsequently, the hydrodynamic and thermal behaviour of the bed was studied using liquid injection. The experimental results revealed that injecting smaller droplets has a larger negative impact on the uniformity of the bed compared to larger droplets. In addition, the injection velocity impacts the average temperature of the bed more with increasing droplet size. Besides the temperature distribution, the IRT can be used to study the agglomerates in the bed as they are visible as dark spots in the IRT-images. The experiments reveal that the formation of agglomerates is more pronounced at increased droplet size. This can be counteracted by an increased solids motion either through a higher background velocity or spout injection velocity. Lastly, the presence of agglomerates was not well reflected in the particle temperature distribution and its properties. Therefore, these are unsuitable to quantify the agglomeration behaviour of the bed.

Finally, the effect of liquid injection on a FBR with porous particles was studied to better represent the above mentioned industrial processes. In the case of porous particles, defluidisation occurs eventually at sufficiently high liquid injection rates due to density driven segregation. For particles with a higher porosity, defluidisation occurs at lower liquid injection rates, as well for particles with a lower pore size. Similar to the agglomeration, the defluidisation due to liquid imbibition can be counteracted by increasing the background fluidisation velocity and the spout velocity.

920 "Separation of Polyolefins by Long-chain Branching (SPOLB)"

In this project a new method for the separation of polyolefins according to the extent of long chain branching (LCB) was elaborated. The polyolefin samples were first separated using size exclusion chromatography (SEC) with the aim to obtain fractions with almost the same hydrodynamic volume. Such macromolecules may differ in their density in the coils, i.e. in their molecular weight, when they differ in the extent of LCB. Temperature gradient interactive chromatography (TGIC) enables a sensitive separation of macromolecules according to their molecular weight, i.e., LCB. The obtained TGIC results indicate separation of the samples according to the molecular weight. Final evidence about separation by LCB will be obtained with SEC- MALLS.

NWO

(CHEMIE.PGT.2017.017)

731.017.414 "Access to chiral acids and amide derivatives with α - and β -stereocenters via copper catalysis"

In dit project hebben we chemische reacties ontwikkeld waarin quinolonen alkynylatie ondergaan onder milde condities. Essentieel voor het slagen van deze reacties is het combineren van katalysatoren gebaseerd op koperzouten met Lewiszuren. De resulterende moleculen hebben een antibacteriële werking en kunnen in de toekomst dus toepassing vinden in geneesmiddelen. Omdat hiervoor meestal één enantiomeer van een werkzaam molecuul nodig is, hebben we ook de enantioselectieve varianten van deze reacties bestudeerd. Onze methode blijkt ook in dit geval goed te werken, wat we gedemonstreerd hebben door middel van succesvolle synthese van cuspareine.

731.017.415 "A program to enable discovery of catalytic and/or allosteric inhibitors of the USP4/11/15 family of deubiquitinating enzymes"

In dit project hebben we meer inzicht verkregen in de enzymwerking van USP15. We hebben ook kristallen gemaakt van het katalytisch domein. Hoewel deze kristallen niet geschikt bleken voor het zoeken naar fragmenten die binden aan het eiwit, gaven ze wel inzicht in de structuur van actieve conformatie van USP15. Daarnaast vonden we een condensaat van mitoxantrone moleculen in dit kristallen, een kristallografische curiositeit, maar eentje die toch ook nieuwe inzichten geeft in condensaat vorming.

731.017.420 "Antisense oligonucleotide therapy, a novel molecular approach to restore CFTR biosynthesis in cystic fibrosis patients"

In CF patiënten is het zout-water transport verstoord waardoor het slijm in de longen taai wordt (taaislijmziekte). Oorzaak van deze erfelijke aandoening is een fout in het DNA, die doorgegeven wordt in het mRNA, wat vertaald wordt naar een defect CFTR-eiwit. In tegenstelling tot de huidige CF medicijnen die op eiwit-nivo werken, is er nu een geneesmiddel in ontwikkeling dat ingrijpt op het mRNA-nivo. Door te onderzoeken hoe manipulaties

omtrent het mRNA en de vertaling daarvan de CFTR structuur en functie beïnvloeden gaan we begrijpen hoe dit nieuwe geneesmiddel werkt, wat nodig is om de ontwikkeling te versnellen en het op termijn te verbeteren. Het afgelopen jaar heeft het onderzoek zich gericht op begrijpen hoe het mRNA de structuur en functie van CFTR kan beïnvloeden. Hiervoor is een aantal verschillende, zogenaamde 'stille' mutaties onderzocht, waarbij de mRNA-code veranderd wordt, maar waarbij deze veranderingen geen invloed hebben op de bouwstenen(volgorde) van de afgelezen eiwitketen. Veranderingen in structuur en functie worden dan alleen maar veroorzaakt door veranderingen in bijv. snelheid van het afleesproces. Alle onderzochte mutaties veroorzaakten verschillen in de productie van CFTR, zelfs al waren de codes van maar 3 tot 5 'letters' (van de 1480) veranderd.