DPI

# Annual Report 2023

# Content





# Organisation 2023

## Supervisory Board

- **Daisuke Ozaki, MSc**
  Chair
- **Dr. Rolf van Benthem**
- **Dr. Krijn Dijkstra**
- **Dr. Lada Kurelec**
- **Arnoud Reininga, MSc**
- **Dr. Erik Van Praet**

## Executive Board

- **Eric Hogenboom**
  Managing Director, Chair
- **Vacancy**
  Scientific Director

## Programme Managers and Business Development

- **Dr. Claude Bostoen**
  Polyolefins
- **Dr. Denka Hristova-Bogaerds**
  Performance Polymers
- **Pooja Jagadeesh, MSc** (left in 2023)
  Business Development
- **Ronald Korstanje, MSc**
  Polymers for Oil and Gas
  Circular Plastics Initiative

## Scientific Programme Chairs

- **Prof.dr. Costantino Creton**
  Performance Polymers
- **Prof.dr. Bernhard Rieger**
  Polyolefins

## Organisation Staff

- **Leon Damen** (left in 2023)
  Project Administration
  Finance
- **Renée Hoogers-Valken**
  Secretariat
- **Peter Kuppens AA**
  Controlling
- **Eylem van Mierlo**
  Finance
- **Rosanne Peters**
  Manager HR&O
- **Christianne Scharff-Bastiaens**
  Communications
- **Linda de Wit**
  Project Administration

# Navigating changes today for tomorrow

**As we reflect on the past year of DPI, it becomes evident that change has become the defining theme of our journey. From the subtle shifts in industry dynamic, the significant ones in policy and economy to the transformations in the organisation. Over the years DPI has remained resilient in the face of challenges while embracing opportunities for growth and innovation. As we stand at the edge of (what seems like yet) another era, it is imperative we examine our role, confront our challenges head-on and navigate changes today for tomorrow.**

## The year that was

I joined DPI as the new managing director in August 2023, but my association with the platform is more than eight years old. We realise that the current times pose new questions for DPI - big and small, challenging as well as inspiring. The market is evolving. The polymer industry is dealing with some setbacks. Some sources of funding seem to be more focused on quicker turnround projects, with traditional long-term research not being a priority. At the same time, new fundamental research projects have been added to the DPI platform, along with new projects for the Circular Plastics Initiative. In our opinion the role DPI plays in facilitating groundbreaking innovation and creating sustainable solutions, for long term challenges, is also more crucial than ever. We strongly believe that industrially driven pre-competitive fundamental polymer research is key to address the most relevant industrial and societal challenges.

## Economic challenges for DPI

The past year has brought forth a perfect storm of challenges for DPI and the broader polymer industry. Rising costs of raw materials and energy, coupled with a shifting funding landscape, have created a turbulent environment.
This is also reflected in the money available for longer-term research. Organisations in the industry have a strong urge to focus on more cost saving, wherever possible, including looking for results and benefits from research in the short-term. DPI's fundamental pre-competitive programme is low TRL (Technology readiness level), which means you cannot implement the findings of the research from these projects in a short time frame. These timelines can, under these circumstances, dissuade more participants from joining DPI's mission.

Since inception, one of the important sources of funding for DPI, has been the Dutch government. However, that stream is also thinning down, due to policy changes. Clearly, we need to secure funding for DPI post-2025. The industry and DPI are in a tough spot, though very gradual signs of recovery may be on the horizon.

## Circular Economy and DPI's Role

Within the last year and in the near future, one trend we can clearly see is a focus shift in the projects under the fundamental programme, towards more sustainability-related solutions. Within the Polyolefins and Performance Polymers programmes more research initiatives are initiated aimed towards solving intriguing issues for meeting longer term industrial sustainability goals.

DPI also remains steadfast in its dedication to promoting sustainability within the polymer industry with the Circular Plastic Initiative, co-founded along with ISPT (Institute for Sustainable Process Technology) in 2019. Our aim is to boost circularity in plastics on an industrial scale, by considering the entire value chain and trying to combat the technological, logistic, and societal challenges facing it. The value chain programme also accounts for higher TRL projects, with technologies or output that can be applied in the plastics production and recycling processes, within a few years.

## Pivot for Progress

As we look to the future, the evolving dynamics requires us to reevaluate our priorities and strategies. Our approach must include further reimagining our research clusters and aligning them with broader industry trends, such as sustainability, energy transition and digitalisation. By doing so we will create a more compelling value proposition for current and future participants and offer them a clearer understanding of the direct benefits to them. Furthermore, categorising research under these themes could also help the programmes fulfil the current criteria for government funding.

## Growth Ambitions

Our ambition is to grow and create a larger impact, with more participants in the ecosystem, both in the low TRL, fundamental programme as well as in higher TRL, value chain projects. We continue to make polymers more effective by designing them for sustainability and contribute to the energy transition. Most of all, we aim to be the most effective industrially driven pre-competitive collaborative platform driving polymer innovation that addresses the most relevant industrial and societal challenges. Keep watching for the next move DPI makes.

ERIC HOGENBOOM

# DPI – Shaping polymer innovation

## DPI fundamental research

Within the fundamental DPI programmes, the research challenges defined by the participating industrial partners are translated by DPI into scientific questions. We invite the most suitable academic groups to propose their ideas on how they can tackle those questions, until proof of concept. The industrial partners decide which ideas will receive grants for further research and they closely follow and guide the scientific output of the project.

DPI aligns the industrial interests and manages the whole process - from defining industrial needs to creating and monitoring relevant research projects. We take care of the day-to-day coordination, while the companies can concentrate their time and efforts on implementing the knowledge gained.

To cover most of the immense spectrum of polymer science, the fundamental research is divided into different programmes. Currently it comprises of the following programmes: Polyolefins, Performance Polymers and Polymers for Oil and Gas.

### Pre-Competitive programme

| Polyolefins | Performance Polymers | Polymers for Oil and Gas |
|---|---|---|
| 17 projects<br>28 researchers | 27 projects<br>40 researchers | 3 projects<br>3 researchers |
| **Industry** | **Industry** | **Industry** |
| • Borealis<br>• Braskem<br>• Dow<br>• ExxonMobil<br>• Reliance Industries Limited<br>• SABIC<br>• SCGC<br>• Shell | • Aramco<br>• Envalior<br>• Hutchinson<br>• Kingfa<br>• SABIC<br>• Shell<br>• SKF<br>• Teijin Aramid | • Shell<br>• SNF |
| **Academia** | **Academia** | **Academia** |
| • Eindhoven University of Technology<br>• Ghent University<br>• INSTM<br>• IPF<br>• Japan Advanced Institute of Science and Technology<br>• Maastricht University<br>• Moscow State University<br>• National Technical University of Athens<br>• Stellenbosch University<br>• University of Chemistry and Technology, Prague<br>• University of Florida<br>• University of Groningen<br>• University of Konstanz<br>• University of Leeds<br>• University of Naples Federico II<br>• University of Perugia<br>• University of Salerno<br>• University of Turin<br>• University of Wisconsin-Madison | • Claude Bernard Lyon 1<br>• Delft University of Technology<br>• Eindhoven University of Technology<br>• ESPCI Paris<br>• Foundation for Research and Technology-Hellas<br>• Ghent University<br>• IFREMER<br>• JOANNEUM RESEARCH<br>• KTH<br>• Maastricht University<br>• Montanuniversität Leoben<br>• National Technical University of Athens<br>• NTNU<br>• Polymer Competence Center Leoben<br>• Radboud University Nijmegen<br>• Shanghai Jiao Tong University<br>• Sichuan University<br>• Southwestern University of Finance and Economics<br>• The University of Edinburgh<br>• Université Savoie Mont Blanc<br>• University of Bologna<br>• University of Crete<br>• University of Lincoln<br>• University of Nottingham<br>• University of Oslo<br>• University of Oxford<br>• University of Patras<br>• University of Twente<br>• VU Amsterdam | • Clausthal University of Technology<br>• Delft University of Technology<br>• University of Groningen |



## Industrial research

The industrial research projects are initiated by DPI, outside of the DPI Fundamental Programmes. Together with industrial and research partners, DPI creates consortia to promote innovation within the value chain. The industrial research projects focus on the further advancement of an innovation and every partner plays an active role. These projects offer companies and research institutes the opportunity to form consortia and to execute innovation activities beyond the proof-of-concept level.

We actively assist in establishing the collaboration and in coordinating the projects. We provide a model framework for this process, while the detailed rules are agreed on between the members of the consortium itself.

### Circular Plastics Initiative

Towards a responsible, circular value chain in plastics
We live in a 'plastic age' where society thrives thanks to developments in polymer science and technology. At the downside, plastic litter can be found all around the globe. As a society, we need to rethink plastic. It is too valuable to be treated as waste. And it can serve as the feedstock for circularity. This calls for concerted action, in particular, to tackle plastic waste and ensure its recycling.

The mission of the Circular Plastics Initiative is to boost circularity in plastics on an industrial scale. We address the entire value chain from an international perspective and focus on the technological, logistic, and societal challenges lying ahead.

Efforts to reduce the use of plastics will contribute to solving its associated problems. However, for many purposes plastics offer advantages to other materials. They often combine high performance with reduced weight and thus help reduce the use of energy. It is therefore equally important to develop a strategy for their responsible use. Circularity will have to be at the heart of this strategy.

At the Circular Plastics Initiative, we work towards a fully circular value chain, from production and use via collecting and sorting towards re-use and recycling. This is done in a concerted action involving all relevant players and addressing all relevant issues. The focus will be in particular on plastics used in food packaging, as these confront us with the most pressing problems. They are prone to irresponsible disposal, they are difficult to sort and it's quite a challenge to bring them back to the beginning of the value chain. Achieving circularity in plastics for food packaging will therefore lead the way to achieving plastics circularity in general.

The Circular Plastics Initiative is co-founded by ISPT and DPI.

Institute for Sustainable Process Technology

**The projects focus on:**

- Analysis of the composition of the mixed plastic waste stream and of contaminants therein
- Evaluation of sorting technology
- Evaluation for chemical processing (pyrolysis & gasification) in terms of quality and scalability (beyond 100 kt/a)
- Evaluation of the opportunities and pitfalls in using the pyrolysis oil as feed for plastic production

**Current projects:**

- CIRCPET – Circular PET trays for perishable food applications
- ReCYCLE – Electrical bike with durable circular plastic parts
- LEMPLAR – Losses & Emissions in Plastic Recycling
- Aramazing
- HOPy – Headstart on pyrolysis
- InReP – An Integrated approach towards Recycling of Plastics
- MPPS – Multipurpose Plastic Sorting

**CPI publication in 2023:**

Juraj Petrík, Homer C. Genuino, Gert Jan Kramer and LI Shen
Pyrolysis of Dutch Mixed Plastic Waste: Lifecycle GHG Emissions and Carbon Efficiency Assessment.

# Summary of financial data 2023

| Income | (x EUR million) | % |
|---|---|---|
| Contributions from industrial partners | 2.81 | 69.5 |
| Subsidy of TKI Toeslag | 0.61 | 15.1 |
| Value chain | 0.44 | 10.9 |
| Business Development | 0.18 | 4.5 |
| **Total income** | **4.04** | **100** |

| Expenditure | (x EUR million) | % |
|---|---|---|
| Personnel costs | 3.38 | 70.1 |
| Depreciation | 0.00 | 0.0 |
| Other costs | 1.00 | 20.8 |
| Value chain | 0.44 | 9.1 |
| **Total expenditure** | **4.82** | **100** |
| **By Programmes** | | |
| Polyolefins | 1.03 | 21.4 |
| Performance Polymers | 1.58 | 32.8 |
| Polymers for Oil and Gas | 0.05 | 1.0 |
| Organisation and support | 1.48 | 30.7 |
| Industrial research | 0.24 | 5.0 |
| Business Development | 0.44 | 9.1 |
| **Total expenditure** | **4.82** | **100** |

# Key Performance Indicators
## DPI fundamental programmes

**Number of industrial partners**

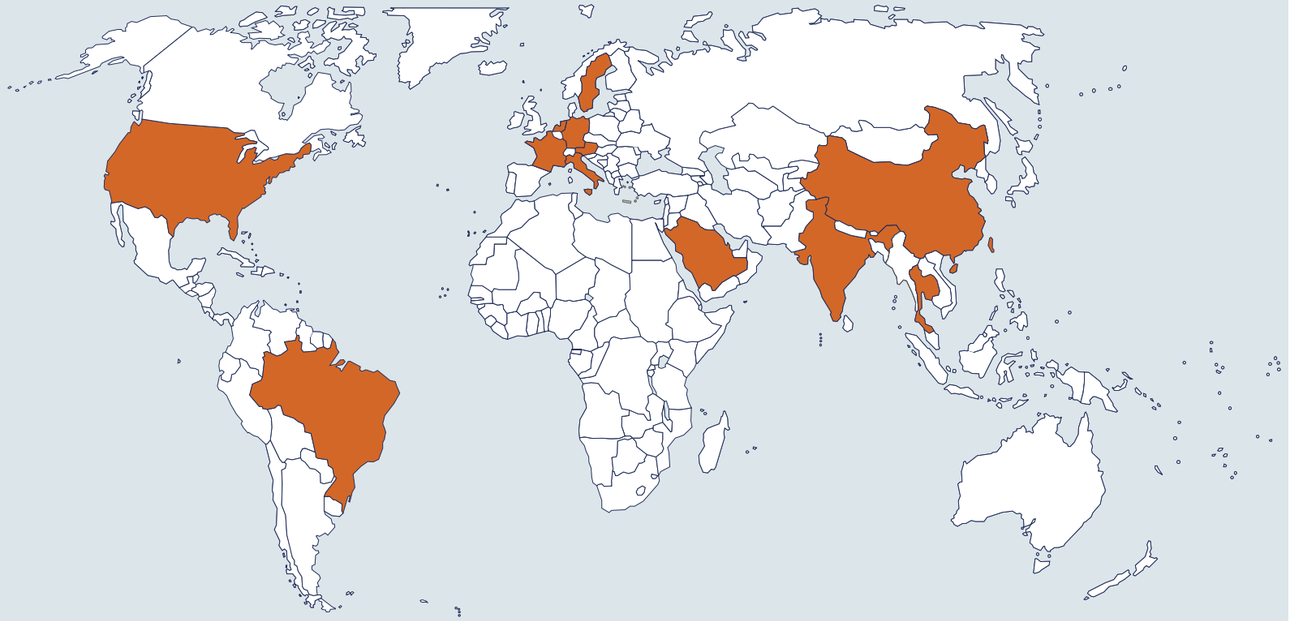

**Number of partner knowledge institutes** (universities, etc.)


| Track record DPI researchers | |
|---|---|
| Left in total | 27 |
| Employed by partner knowledge institute | 14 |
| Employed by non-partner knowledge institute | 0 |
| Employed by partner industrial company | 2 |
| Employed by non-partner industrial company or start-up | 8 |
| Unknown | 3 |

| Research output | 2022 | 2023 |
|---|---|---|
| Scientific publications | 25 | 31 |
| PhD theses | 4 | 14 |
| Average journal impact factor | 5.47 | 6.7 |

# Partners industry 2023

**involved in DPI fundamental programmes**



## Europe

| | |
|---|---|
| Borealis | BOREALIS Keep Discovering |
| Hutchinson | HUTCHINSON |
| SKF | SKF |
| SNF Floerger | SNF WATER SCIENCE |

## The Netherlands

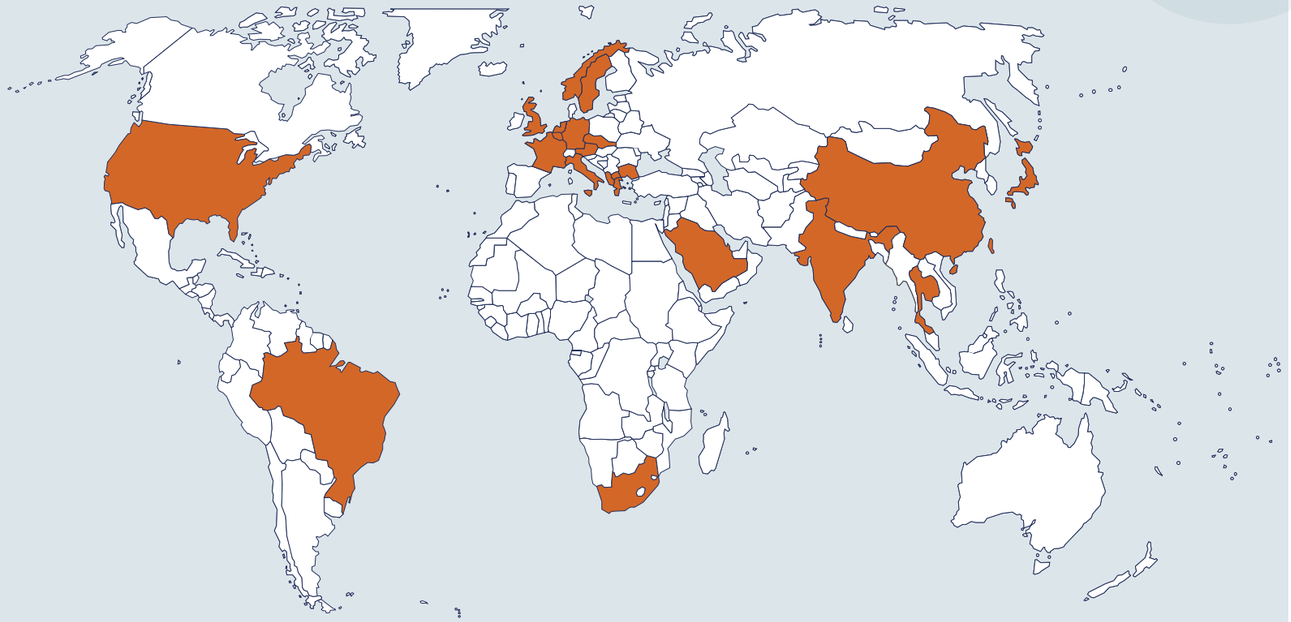
| | |
|---|---|
| Dow Benelux | DOW |
| Envalior | Envalior Imagine the Future |
| SABIC | سابك sabic |
| Shell | |
| Teijin Aramid | TEIJIN |

## North and South America, Asia

| | |
|---|---|
| Aramco | aramco |
| Braskem | Braskem |
| ExxonMobil | ExxonMobil |
| Kingfa | KINGFA |
| Reliance Industries Limited | Reliance Industries Limited |
| SCG Chemicals | SCGC |

# Partners knowledge institutes 2023

**involved in DPI fundamental programmes**



## Europe

- Claude Bernard Lyon 1
- ESPCI Paris
- Foundation for Research and Technology - Hellas
- Ghent University
- IFREMER
- INSTM
- IPF
- JOANNEUM RESEARCH
- KTH
- Montanuniversität Leoben
- National Technical University of Athens
- NTNU
- Polymer Competence Center Leoben
- University of Edinburgh
- TU Clausthal
- University Savoie Mont Blanc
- University of Bologna
- University of Chemistry and Technology Prague
- University of Crete
- University of Konstanz
- University of Leeds (new in 2023)
- University of Lincoln
- University of Naples Federico II
- University of Nottingham
- University of Oslo
- University of Oxford
- University of Patras
- University of Perugia
- University of Salerno
- University of Turin

## Netherlands

- Delft University of Technology
- Eindhoven University of Technology
- Maastricht University
- Radboud University
- University of Groningen
- University of Twente
- VU Amsterdam

## North and South America, Asia

- Japan Advanced Institute of Science and Technology
- Shanghai Jiao Tong University
- Sichuan University
- Southwestern University of Finance and Economics
- Stellenbosch University (new in 2023)
- University of Florida (new in 2023)
- University of Wisconsin-Madison

# Polyolefins

The Polyolefins research programme encompasses the entire spectrum of the knowledge chain. The aim is to create the knowledge base necessary to support an ever-expanding range of applications.
Polyolefin-based materials can be customised for many different applications: from ultra-rigid thermoplastics to high-performance elastomers. This wide range of performance is achieved due to a variety of polyolefin molecular structures that share common features of high atomic efficiency in synthesis, low cost, excellent properties, long lifetime, and easy recyclability.
The mission of this Programme is to support and coordinate integrated pre-competitive or explorative research projects, on polyolefins, along the whole knowledge chain. From (homogeneous and heterogeneous) catalyst synthesis and immobilisation, through catalytic olefin polymerisation, down to polyolefin characterisation, processing, and end-use evaluation. Care for materials and process sustainability, from the perspective of a Circular Economy, is a pervasive characteristic of the research Programme.

## Focus areas

### Circular Economy solutions for Polyolefins

The The key focus of this sub programme is on mechanical recycling and chemical recycling processes, non-chemical recycling, and non-mechanical methods of recycling, while preserving quality and purity of recyclates. The aim is to develop a new concept of recycling design especially based on polyolefins, among others, to circumvent the multi-layer complexity of PET/EVOH/PE composites. Either through polymer design or specific processing steps, with adjusting $O_2$/$CO_2$ barrier properties. Polyolefin modification based on renewable sources is another route to establishing these circular economy targets.

### Polymer structure, properties and processing

Understanding, modelling and predicting structure-processing property relationships in polyolefin-based polymer systems.

### Polymer reactor engineering

Studying various reactor and technology unit operations to develop a quantitative description and acquire a thorough understanding of the crucial aspects of olefin polymerisation processes.

### New methods and exploratory research

New polymerisation and polymer characterisation methods, high-throughput screening and experimentation, embryonic research and concept development.

### Catalysis

Investigating, screening and developing (novel) homogeneous and heterogeneous catalyst systems, as well as new approaches for the immobilisation of molecular catalysts, new co-catalysts and activators. .

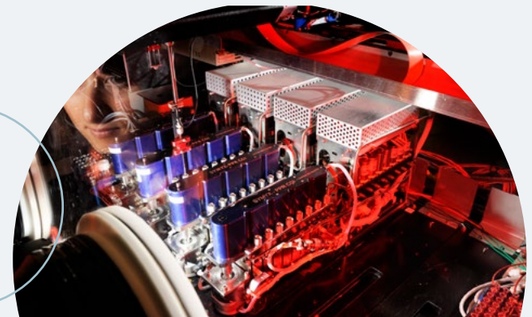
## Facts and figures

### Partners from industry

- Borealis
- Braskem
- Dow
- ExxonMobil
- Reliance Industries Limited
- SABIC
- SCGC
- Shell

### Partners from the research world

- Eindhoven University of Technology
- Ghent University
- INSTM
- IPF
- Japan Advanced Institute of Science and Technology
- Maastricht University
- Moscow State University
- National Technical University of Athens
- Stellenbosch University
- University of Chemistry and Technology, Prague
- University of Florida
- University of Groningen
- University of Konstanz
- University of Leeds
- University of Naples Federico II
- University of Perugia
- University of Salerno
- University of Turin
- University of Wisconsin-Madison



### Budget and organisation

In 2023 there were 28 researchers (PhDs and postdocs) working within the 17 projects of the Polyolefins programme, 2 new projects started with a total budget of €0.4 Million. Prof.dr. Bernhard Rieger was Scientific Chair and Dr. Claude Bostoen was Programme Manager.

### Publications and inventions

This programme generated 16 reviewed papers, 5 theses in 2023 and one reported invention.

For details, see page 18

# Performance Polymers

Performance Polymers possess superior chemical, mechanical and physical properties, especially beyond ambient conditions. They are typically used as multi-component polymeric systems consisting of various polymers, reinforcements and additives.

The research focus of the Performance Polymers Programme is on enhancing the performance of advanced polymeric systems, by combining Chemistry, Physics and Engineering Science, using state-of-the art modelling and characterisation tools. This leads to a better understanding and predicting of the “structure versus performance” relation and of the lifetime of the performance polymers, and contributes to the design of new/improved performance materials of the future.

The knowledge generated through this programme provides opportunities for responding to the new sustainability challenges. Especially for the automotive, aerospace, electronics, oil & gas transport, energy and construction industrial sectors.

## Focus areas

### Advanced modelling & experimental strategies for enhanced durability & performance

- Surface treatment for enhanced polymer performance
- Composites fatigue: prediction of damage and correlation to lifetime
- Impact mechanisms in polymer composites
- Extending durability / lifetime of performance polymers
- Advances in solid-state NMR for polymeric systems

### Processing – Structure – Performance relationship

- Flow instability and processing of filled polymeric melts
- Linking rheology to the molecular and macroscopic structure of polymers

### Polymers for electronics and energy storage/ transportationy

- Informed design of electrically conductible composites
- Polymers and composites under high voltage conditions
- Polymers as high-barrier materials for gas (H2) storage/ transportation
- Polymers for solid state batteries

### Recycling / Reprocessing / Recovery of performance polymers

- Reversible bonds for re-use/recycling of composites and thermosets
- Composites recycling / re-processing

### Alternative resources for performance polymers

- Bio-based polyamides
- $CO_2$ derived polymers

## Facts and figures

### Partners from industry

- Aramco
- Envalior
- Hutchinson
- Kingfa
- SABIC
- Shell
- SKF
- Teijin Aramid

### Partners from the research world

- Claude Bernard Lyon 1
- Delft University of Technology
- Eindhoven University of Technology
- ESPCI Paris
- Foundation for Research and Technology-Hellas
- Ghent University
- IFREMER
- JOANNEUM RESEARCH
- KTH
- Maastricht University
- Montanuniversität Leoben
- National Technical University of Athens
- NTNU
- Polymer Competence Center Leoben
- Radboud University Nijmegen
- Shanghai Jiao Tong University
- Sichuan University
- Southwestern University of Finance and Economics
- The University of Edinburgh
- Université Savoie Mont Blanc
- University of Bologna
- University of Crete
- University of Lincoln
- University of Nottingham
- University of Oslo
- University of Oxford
- University of Patras
- University of Twente
- VU Amsterdam

### Budget and organisation

In 2023 there were 40 researchers (PhDs and postdocs) working within the 27 projects of the Performance Polymers programme, 3 new projects started with a total budget of €1.05 Million. Prof.dr. Costantino Creton was Scientific Chair and Dr. Denka Hristova-Bogaerds was Programme Manager of the Performance Polymers programme.

### Publications

This programme generated 14 reviewed papers and eight theses in 2023. For details, see page 19

# Polymers for oil and gas

Polymers find broad application in the recovery, transport and utilisation of oil and gas. For example, as oil field chemicals or as lightweight materials with superior durability properties. The Polymers for Oil and Gas programme aims to generate tools and new insights into existing and new polymers, for utilisation in the exploration, production and transport of oil and gas. The focus is on two main areas of study. The first is the use of polymers in fluids for enhanced oil recovery (EOR) and other sub surface drilling/recovery applications. Second, polymer behaviour in functional materials used under extreme/adverse conditions (in close collaboration with the Performance Polymers programme).

## Focus areas

### Structure–property relationships and the design of new model macromolecules

Controlled radical polymerisation techniques will be employed to investigate the effects of macromolecular topology. For example, branching, on polymer solution properties and on viscosity and/or visco-elasticity. These novel structures are evaluated in core flow experiments to determine their injectivity and impact on the recovery of oil in porous media. The effects of polymeric surfactants, i.e. high molecular weight amphiphilic structures, that have the potential to decrease the interfacial tension and enhance oil recovery, are also being investigated. These may yield better results compared to those obtained with the current polymer flooding applications.

### Relating polymer rheology to apparent viscosity in porous media

Developing reliable models to predict the relationship of polymer-apparent viscosity in porous media to porous-medium properties, bulk rheological parameters, and superficial velocity in the medium, and establish the relationship with enhanced oil recovery.

The programme was terminated in 2023 as there is no longer a need for fundamental research.

## Facts and figures

### Partners from industry

- Shell
- SNF



### Partners from the research world

- Delft University of Technology
- TU Clausthal
- University of Groningen

### Budget and organisation

In 2023 there were 3 researchers (PhDs and postdocs) working within 3 projects of the Polymers for oil and gas programme. Ronald Korstanje acted as Programme Manager.

### Publications and inventions

This programme generated 1 master thesis in 2023.
For details see page 21

# Output

## Polyolefins

### Projects

**#804:** From homogeneous to “colloidal” olefin polymerization catalysts: effects of mass transport limitations on reaction kinetics and polymer microstructure

**#813:** Multi-scale investigation of silica-supported ethylene polymerization catalysts during the early stages of the reaction

**#830:** Electrostatic charging of polyolefin powders on the level of particles

**#831:** Molecular modelling of stretch-induced crystallization in polyethylene and polypropylene layers

**#832:** Quality model for COntaminated Recycled Polyolefins

**#834:** RHEOlogical determination of POLyolefin ARchitectures

**#835:** Quantitative Structure-Activity Relationships (QSAR) in Post-Metallocene-Based Olefin Polymerizations Using Chemically Meaningful Computational Descriptors

**#836:** Practical, High Throughput Quench Labeling Techniques for Information-Rich Analysis of Alkene Polymerization Catalysts

**#846:** In-Chain Functionalized Polyethylenes from Controlled Free-Radical Polymerization under Benign Conditions

**#847:** A microstructural insight in polyethylene based bioriented mono-materials: from fundamental to processing

**#848:** Ziegler-Natta Catalysts for Polypropylene with Temperature-Controlled ID/ED Compositions

**#855:** Governing Sparsely Long Chain Branching in Polyolefins by rheology: a milligram size approach

**#856:** Multi-scale Analysis and Design of the Pyrolysis of Polyolefins

**#857:** Innovative Molecular Activators for Olefin Polymerization

**#858:** High Temperature Thermal Field Flow Fractionation: Meeting the Challenges in Advanced Characterization of Branching and Ultra-High Molar Mass Distributions in Polyolefins – A Feasibility Study.

**#861:** Closing the Loop via Molecular Polymer Rheology (started in 2023)

**#863:** Machine-Learning-aided 13C NMR/CEF rapid analysis of polyolefin materials, with special focus on post-consumer streams (started in 2023)

### Theses

**Vincenzo Ianniello**
Rheological Determination of Polyolefin Architecture

**Stan Looijmans**
Adhesion-modified polypropylene composites: a sticky situation

**Federico Di Sacco**
Structural transition of polypropylenes during cast film extrusion, heating and confinement

**Max Werny**
Probing the Morphology, Composition and Temperature of Olefin Polymerization Catalyst Particles with Microscopy and Spectroscopy

**Jelena Zarupski**
Spectroscopic characterization of silica-supported ethylene polymerization catalysts

### Publications

A. Vittoria, P.S. Kulyabin, G. Antinucci, A.N. Iashin, D.V. Uborsky, E.N.T. Cuthbert, P.H.M. Budzelaar, A.Z. Voskoboynikov, R. Cipullo, C. Ehm and V. Busico
*The Interplay of Backbone Stiffening and Active Pocket Design in Bis(phenolate-ether) Zr/Hf Propene Polymerization Catalysts*
Acs Catalysis 13 (20) 13151-13155

M.J. Werny, F. Meirer and B.M. Weckhuysen
*Visualizing the Structure, Composition and Activity of Single Catalyst Particles for Olefin Polymerization and Polyolefin Decomposition*
Angewandte Chemie-International Edition

M. Milanesi, A. Piovano, T. Wada, J. Zarupski, P. Chammingkwan, T. Taniike and E. Groppo
*Influence of the synthetic procedure on the properties of three Ziegler-Natta catalysts with the same 1,3-diether internal donor*
Catalysis Today 418

A. Dall’Anese, P.S. Kulyabin, D.V. Uborsky, A. Vittoria, C. Ehm, R. Cipullo, P.H.M. Budzelaar, A.Z. Voskoboynikov, V. Busico, L. Tensi, A. Macchioni and C. Zuccaccia
*Octahedral Zirconium Salan Catalysts for Olefin Polymerization: Substituent and Solvent Effects on Structure and Dynamics*
Inorganic Chemistry 62 (39) 16021-16037

D.V. Uborsky, M.I. Sharikov, G.P. Goryunov, K.M. Li, A. Dall’Anese, C. Zuccaccia, A. Vittoria, T. Iovine, G. Galasso, C. Ehm, A. Macchioni, V. Busico, A.Z. Voskoboynikov and R. Cipullo

*Manipulating pre-equilibria in olefin polymerization catalysis: backbone-stiffening converts a living into a highly active salan-type catalyst*
Inorganic Chemistry Frontiers 10 (21) 6401-6406

J. Zarupski, A. Piovano, M.J. Werny, A. Martini, L. Braglia, P. Torelli, C. Hendriksen, N.H. Friederichs, F. Meirer, B.M. Weckhuysen and E. Groppo
*Silica-magnesium-titanium Ziegler-Natta catalysts. Part II. Properties of the active sites and fragmentation behaviour*
Journal of Catalysis 423 10-18

J. Zarupski, A. Piovano, M. Signorile, A. Amodio, L. Olivi, C. Hendriksen, N.H. Friederichs and E. Groppo
*Silica-magnesium-titanium Ziegler-Natta catalysts. Part 1: Structure of the pre-catalyst at a molecular level*
Journal of Catalysis 424 236-245

R.L. do Rosario, F. Christakopoulos, T.A. Tervoort, F. Brunel and T.F.L. McKenna
*Gas-phase polymerization of ultra-high molecular weight polyethylene with decreased entanglement density*
Journal of Polymer Science 61 (12) 1183-1195

G. Urciuoli, O.R. de Ballesteros and F. Auriemma
*Molecular Architecture of Multiblock Copolymers Synthesized by the Chain Shuttling Technology*
Macromolecular Chemistry and Physics

S.F.S.P. Looijmans, D. Cavallo, D.H. Merino, J.C. Martinez, P.D. Anderson and L.C.A. van Breemen
*Shear-Induced Structure Formation in MAH-g-PP Compatibilized Polypropylenes*
Macromolecules 56 (14) 5278-5289

N.I. Sigalas, S.A.T. Van Kraaij and A.V. Lyulin
*Effect of Temperature on Flow-Induced Crystallization of Isotactic Polypropylene: A Molecular-Dynamics Study*
Macromolecules 56 (21) 8417-8427

G. Urciuoli, A. Vittoria, F.D. Cannavacciuolo, R. Cipullo, S. Costanzo, V. Ianniello, F. Bellavista, O.R. de Ballesteros, V. Busico, N. Grizzuti and F. Auriemma
*Effect of Segregation Strength on Mesophase Separation in Statistical Multiblock Copolymers Synthesized through a High-Throughput Experimentation Approach*
Macromolecules 56 (24) 10163-10178

V. Ianniello, S. Costanzo, R. Pasquino, G. Ianniruberto, V.K. Gupta, L. Stieglitz, B. Rieger, T. Tervoort and N. Grizzuti
*Evaluating the molecular weight distribution of ultrahigh molecular weight polypropylene through rheology*
Physics of Fluids 35 (6)

F. Di Sacco, E. Solano, M. Malfois, J.B. Wang, M. Gahleitner, R. Pantani and G. Portale
*Real-time structural characterization of isotactic polypropylene during cast film extrusion*
Polymer 276

S.F.S.P. Looijmans, H. Ahmadi, P.D. Anderson and L.C.A. van Breemen
*Deformation kinetics of single-fiber polypropylene composites: Adhesion improvement at the expense of toughness*
Polymer 286

G. Urciuoli, F. Zaccaria, C. Zuccaccia, R. Cipullo, P.H.M. Budzelaar, A. Vittoria, C. Ehm, A. Macchioni and V. Busico
*A Hydrocarbon Soluble, Molecular and “Complete” Al-Cocatalyst for High Temperature Olefin Polymerization*
Polymers 15 (6)

### Reported invention

**#858:** Martin Geisler and Albena Lederer
High Temperature Thermal Field Flow Fraction

## Performance Polymers

### Projects

**#811:** Reliable Prediction of Residual Structural Integrity and Damage-Evolution During Long-Term Fatigue in Thermoplastic Composites

**#812:** Physics-based fatigue design tool for matrix cracking and delamination in unidirectional and sandwich composites under multi-axial fatigue loads with arbitrary R-ratio: development, validation and finite element implementation

**#823:** Modular, designer polydopomine adhesives for facile and versatile surface conjugation of function of polyethylenes

**#824:** Micromechanical modelling of complex composite systems for improved failure prediction and product design

**#825:** Development of Hyperpolarized and 1H MAS NMR Spectroscopy for the study of performance polymers

**#826:** Multi-layered wEar-Resistant Coatings with additional fUnctionality – new stRategies for enhancIng the tribologicAl performance of poLymers in demanding environments

**#827:** Impact Modelling of Polymers: high-Rate Experiments for Solid-state Simulations

**#828:** Elastomer DEgradation under MEchanical Loading: investigation of coupling effect

**#829:** Physical and chEmical Ageing of amoRphous polymers by moLecular simulation

**#837:** Linking rheological material functions to polymer crystallization

**#838:** Supramolecular modulation of the network connectivity in vitrimers

**#839:** Dynamic chemistry for tunable reversible bonding in bulk and at interfaces

**#840:** Engineering the rheology ANd processinG-induced structural anisotropy of poLymEr composites with non-Brownian fibrous particles

**#841:** Understanding the Rheological Origin of Striped Flow Marks in Injection Molding

**#843:** Recyclable high-performance composites with reversible interface bonding

**#844:** Modelling and Design of Multiphase Polymeric Materials for High Performance Applications Across Multiple Scales

**#845:** A joint molecular modelling and experimental approach to developing novel thin-film polymer barriers for gas containment systems

**#850:** Mechanism of Electrical Aging Caused by Different Structural Defects in Performance Polymer Materials

**#851:** Creep Fatigue Interaction in Performance Polymers at High Temperatures

**#852:** Thermo-electrical ageing mechanisms in polymer-ceramic nanocomposites for energy storage applications

**#853:** PA/Glass fiber recycling by reactive extrusion

**#854:** Monitoring lifetime of thermoplastic composites by combining analytics and machine learning

**#859:** Quantum-Chemical Life-Time Optimization of Sustainable Engineering Polymers

**#860:** OptimiseD matrix and fIbre treatmeNt for high performance thermoplastic composites recycling

**#864:** Biobased crystal polarization and semi-aromaticity for high polymer dielectrics (started in 2023)

**#865:** Engineering Polymers from CO2 using advanced switchable catalysis (started in 2023)

**#866:** Achieving high-energy solid-state batteries with succinonitrile-based electrolytes (started in 2023)

## Theses

**Thanasis Athanasiou**
Rheometric tools and protocols for materials with multi-scale response and fading mechanical memory

**Meryll Barraco**
Development of a thin-film polymer barrier on a dense substrate by using interfacial polymerization combined with molecular modelling – Application to high-pressure hydrogen storage tanks

**Yubao Deng**
Simulation of Percolation in Nanocomposite Materials Systems

**Josef Sommer**
Experimental study of the damage behaviour of thermoplastic glass/polypropylene laminates under in-plane tension fatigue

**Alvaro Quinteros Sedano**
Covalent and non-covalent approaches to modulate the viscoelastic and mechanical properties of boronic ester-based vitrimers

**Peihao Song**
Strain Rate, Temperature, and Their Coupled Effects on the Deformation Process of Four Polycarbonates and a Short Glass Fibre Reinforced Polycarbonate Composite

**Sabrina Taourit**
Chemical degradation of elastomers under mechanical loading: study of a coupling effect

**Martijn Wismans**
Multiaxial Failure of Short-fiber Reinforced Thermoplastics

## Publications


R. Milatz, J. Duvigneau and G.J. Vancso
Dopamine-Based Copolymer *Bottlebrushes for Functional Adhesives: Synthesis, Characterization, and Applications in Surface Engineering of Antifouling Polyethylene*
Acs Applied Materials & Interfaces 15 (28) 34023-34030

A. Sexton, M. Kanters, H. Demchenko, B. Pacáková, J.O. Fossum, L. Balzano and M. Knaapila
*Classifying Tensile Loading History of Continuous Carbon Fiber Composites Using X-Ray Scattering and Machine Learning*
Advanced Engineering Materials

M.A. Bissett, Y.B. Deng, I.A. Kinloch and W.W. Sampson
*Percolation Threshold of Clustered, Oriented and Polydisperse Sticks in a Plane*
Advanced Theory and Simulations

J. Sommer, M. Hajikazemi, I. De Baere and W. Van Paepegem
*Fatigue behaviour of thermoplastic glass/polypropylene composite cross-ply laminates: An experimental study with in-situ damage observations and numerical validation*
Composites Part B-Engineering 252

J. Sommer, M. Hajikazemi, I. De Baere and W. Van Paepegem
*Experimental and numerical fatigue damage characterization in multidirectional thermoplastic glass/polypropylene laminates based on in-situ damage observations*
Composites Part B-Engineering 267

O. Atiq, E. Ricci, M.G. Baschetti and M.G. De Angelis
*Multi-scale modeling of gas solubility in semi-crystalline polymers: bridging Molecular Dynamics with Lattice Fluid Theory*
Fluid Phase Equilibria 570

H.S. Siebe, A.S. Sardjan, S.C. Massmann, J. Flapper, K.J. van den Berg, N.N.H.M. Eisink, A.P.M. Kentgens, B.L. Feringa, A. Kumar and W.R. Browne
*Formation of substituted dioxanes in the oxidation of gum arabic with periodate*
Green Chemistry 25 (10) 4058-4066

M. Wismans, S.J.J. van den Broek, L.C.A. van Breemen, L.E. Govaert and T.A.P. Engels
*Micromechanical analysis of age-induced strength reduction in a multiaxially loaded short-fiber reinforced thermoplastic*
Journal of Applied Polymer Science 140 (41)

M. Barraco, S. Neyertz, N.E. Benes and D. Brown
*Comparison of Eight Classical Lennard-Jones-Based H*
Journal of Physical Chemistry A 127 (30) 6335-6346

C.C. Zhang, Y.M. Li, K. Zhou, J.L. Yang and G.X. Li
*Crystal structure-flashover performance correlation in polybutylene terephthalate: Insights into the mechanism*
Journal of Polymer Science

S. Taourit, P.Y. Le Gac and B. Fayolle
*Coupling between hydrolysis and mechanical relaxation in an ester-based polyurethane network*
Journal of Polymer Science 61 (22) 2892-2900

A. Aerts, S.F.S.P. Looijmans, L.C.A. van Breemen, R.P. Sijbesma and J.P.A. Heuts
*Fluorescent Visualization of Bond Breaking in Polymer Glasses*
Macromolecules 56 (11) 4267-4277

G.G. Vogiatzis, L.C.A. van Breemen, M. Huetter and D.N. Theodorou
*Network dynamics: a computational framework for the simulation of the glassy state*
Molecular Systems Design & Engineering 8 (8) 1013-1029

P.H. Song, A.R. Trivedi and C.R. Siviour
*Mechanical response of four polycarbonates at a wide range of strain rates and temperatures*
Polymer Testing 121


## MSc thesis

**Aniket Modi**
Simulation and history-matching of polymer-assisted water alternating CO2 injection using MRST

# NEWPOL

## Publication

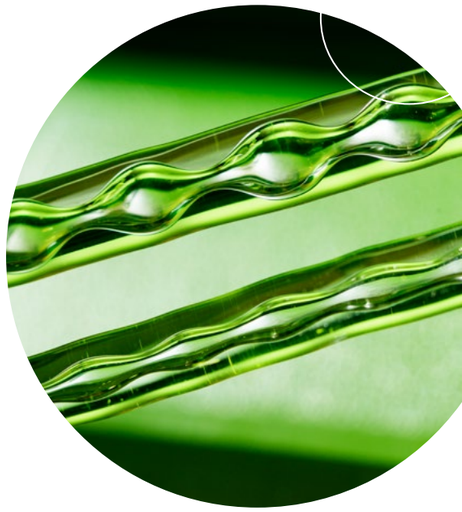

I. Maric, L.L. Yang, X.F. Li, G.M. Santiago, C.G. Pappas, X.K. Qiu, J.A. Dijksman, K. Mikhailov, P. van Rijn and S. Otto
*Tailorable and Biocompatible Supramolecular-Based Hydrogels Featuring two Dynamic Covalent Chemistries*
Angewandte Chemie-International Edition


# Polymers for Oil and Gas

## Projects

**#818:** Experimental and Numerical Evaluation of Polymer Viscoelasticity Effects during EOR Applications

**#821:** New Polymeric Surfactants for Enhanced Oil Recovery
**#849:** Feasibility study of enhanced oil recovery by Polymer Assisted Water-Alternating-Gas



# DPI

DPI is a foundation funded by industry, universities and the government which was set up to perform exploratory research in the area of polymer materials.

DPI operates at the interface of universities and industry, linking the scientific skills of university research groups to the industrial need for innovation.

DPI carries out pre-competitive research projects to add value to the scientific community through scientific publications and to the industrial community through the creation of intellectual property.

DPI provides a unique platform for generating awareness of new technology, in which participating industrial companies, competitors in the market place, communicate on a pre-competitive basis to trigger innovation.

DPI integrates the scientific disciplines and know-how of universities into the ‘chain of knowledge’ needed to optimise the conditions for making breakthrough inventions and triggering industrial innovation.

DPI aims to combine scientific excellence with a genuinely innovative impact in  industry, thereby creating a new mindset in both industrial and academic research.

DPI aims to fill the innovation gap between industry and universities and so resolve the Dutch Paradox of scientific excellence and lack of innovation.

Some 80 researchers (PhDs and Post-Docs) are currently involved in DPI projects at knowledge institutes throughout the world.

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