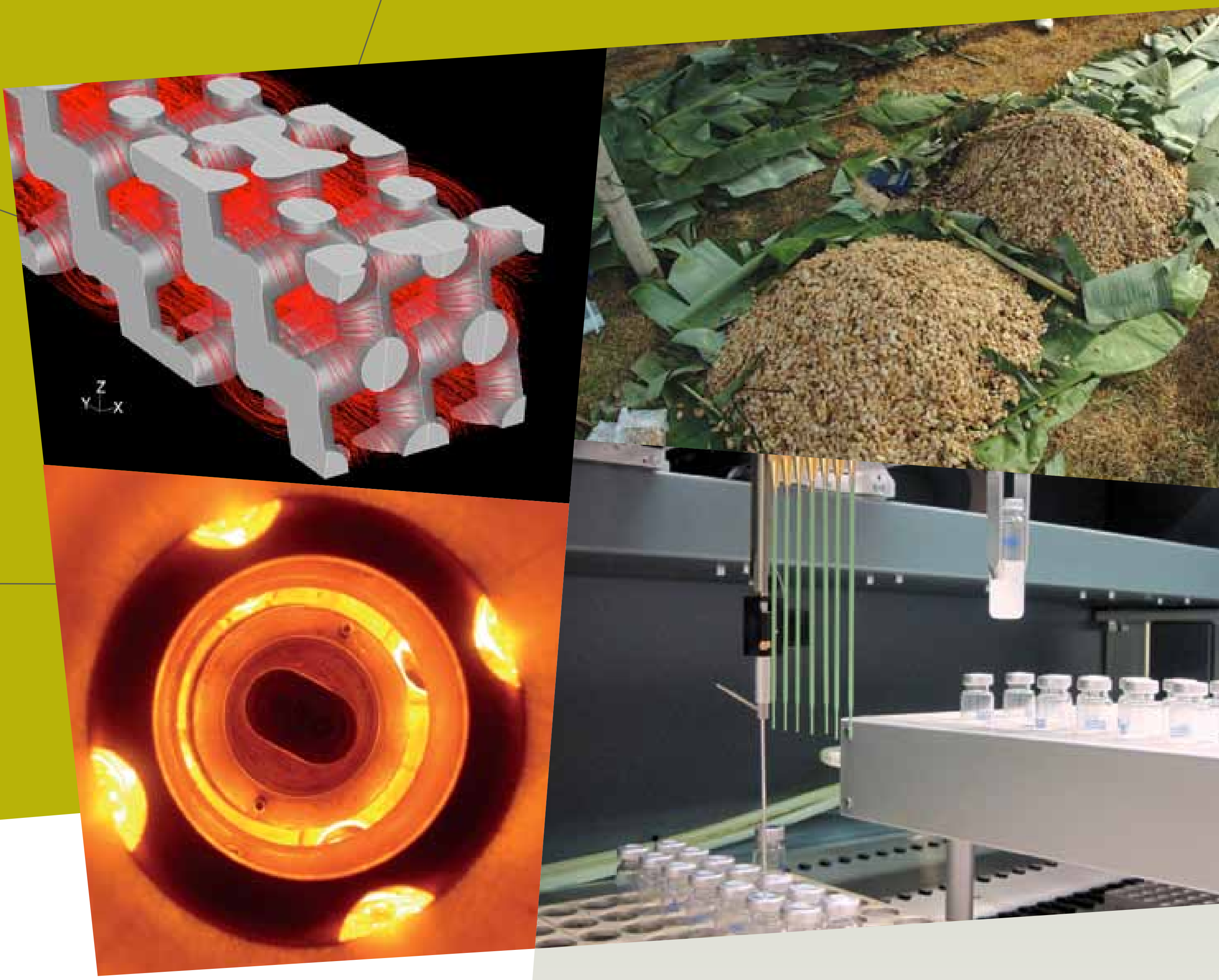

Vrije
Universiteit
Brussel

Sustainable Chemistry
Research

PUBLISHER'S IMPRINT

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Cover photographs
Clockwise:
CHIS - Simulation of flow patterns in a structured microreactor
IMDO - Cocoa bean heap fermentation
CHIS - High-throughput evaluation of adsorbents for solvent purification
FYSC - Heat-cool DSC infrared heating for rapid scanning

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Towards the era of sustainable chemistry

Our society is facing great challenges regarding the use of natural resources, energy production and consumption, and the provision of food, water and healthcare to its population. **Chemistry, Materials and Life Sciences are essential for making the world's development sustainable**. Consequently it is crucial for innovative research to focus on the sustainable development of new products, applications and services.

The mission of **Flanders Innovation Hub for Sustainable Chemistry (FISCH)** is to catalyze the transition of Flanders' broad chemical industry to an era of sustainable chemistry. The FISCH competence pool is an initiative of essencia flanders – the multisectoral umbrella organization representing the numerous sectors of activity in the field of chemicals and life sciences –, VITO (Flemish Institute for Technological Research), chemical producing industries, downstream users of chemicals and the Flemish Universities. The aim of FISCH is the realization of an innovative and strategic platform for sustainable chemistry.

Sustainable chemistry relates to the contribution of chemistry – in its broadest sense – across all areas of sustainable development, including:

- Efficient conversion and rational use of natural resources
- Search for new and sustainable resources to produce chemicals and energy
- Development of hyperselective biochemical processes
- Intensification of existing energy intensive processes
- Recycling and valorization of waste streams
- Development of sustainable business models
- And many others

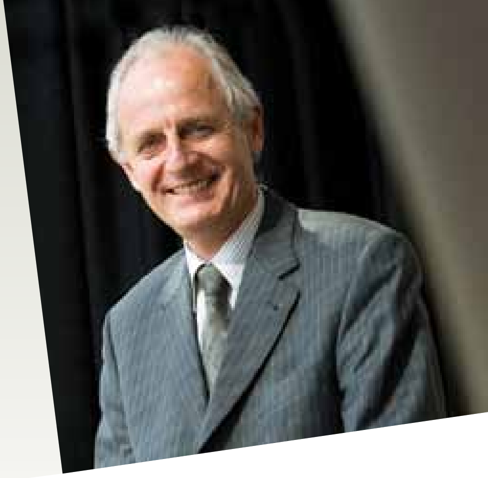
FISCH will enhance the development of sustainable chemistry through the **reinforcement of competences in companies, universities and knowledge centers** and through the **clustering of existing knowledge, innovation platforms and infrastructures**. This will create new value chains and enable FISCH to maintain a world-leading position.

To achieve this ambition, the FISCH competence pool will support different types of projects, including:

- Innovation program roadmaps
- Systemic projects stimulating collaboration between companies to generate new activities
- Collective research projects
- Open innovation structure projects for research or upscaling

To facilitate a fruitful collaboration between companies, knowledge centers and universities in sustainable chemistry research, the inventorying of existing know-how is indispensible. This brochure provides an **overview of competences at the Vrije Universiteit Brussel in relation to sustainable chemistry**. We hope this will open up new routes towards a sustainable society.

Joeri Denayer
Professor at the Department of Chemical Engineering
Vrije Universiteit Brussel



Innovating for greater resource efficiency

FISCH
The innovation platform for sustainable chemistry in Flanders
www.suschem.be

A feasibility study conducted among the chemical and life sciences sector and potential partners led to the setting up of the FISCH platform. FISCH stands for **'Flanders Innovation Hub for Sustainable Chemistry'** and its aim is **to drive the transition of industries in the chemical value chain to become sustainable.** From January 2012, FISCH has been recognized as a competence pool by the Flemish government. Sustainable chemistry spearheads the 'New Industrial Policy for Flanders' white paper approved by the Flemish government in May 2011. FISCH has been approved by SusChem Europe, the EU commission-chemical sector sustainable chemistry technology platform, giving FISCH international visibility and creating new opportunities for cooperation.

Mission and strategy
FISCH's mission is to enhance innovations in the field of sustainable chemistry and bring them to market more quickly, thus speeding up the sector's move to sustainability. In this way, industry creates new value chains, and contributes towards its global competitiveness; FISCH is intended to reinforce Flanders' position among Europe's leaders in sustainable chemistry.
FISCH's main aim is twofold:

- To develop new value chains based on sustainable chemistry in the disciplines outlined in its strategic innovation agenda
- To build collective and cooperative sustainable chemistry skills to enable these new value chains

The FISCH logo – a ferryboat with three sails – symbolises this three-pronged strategy:

- A strategic innovation agenda for sustainable chemistry
- An enabling open innovation infrastructure cluster
- A sustainable chemistry knowledge centre

Strategic innovation agenda for sustainable chemistry
FISCH has selected nine of the 80 research topics covered by SusChem Europe and groups companies, knowledge institutions and universities into consortiums under three 'breakthrough domains':

- Alternatives to fossil fuels
- Process intensification
- Sustainable chemical products and processes

Open innovation infrastructure cluster
The implementation of innovative sustainable chemistry projects requires high-tech and often expensive infrastructures to facilitate the whole process including, for example, up-scaling. The FISCH open innovation infrastructure cluster will list, group together, manage and optimise all available innovation equipment. The infrastructure will be made available to participating companies, knowledge centres and universities.

Sustainable chemistry knowledge centre
The sustainable chemistry knowledge centre will combine all existing efforts and skills with a view to creating a database for research and development which will be circulated among sustainable chemistry stakeholders. To achieve this objective, FISCH is cooperating with existing knowledge centres and institutes of higher education to provide complementary activities. The knowledge centre will strive to promote and facilitate the initiation and development of new value chains for sustainable chemistry.

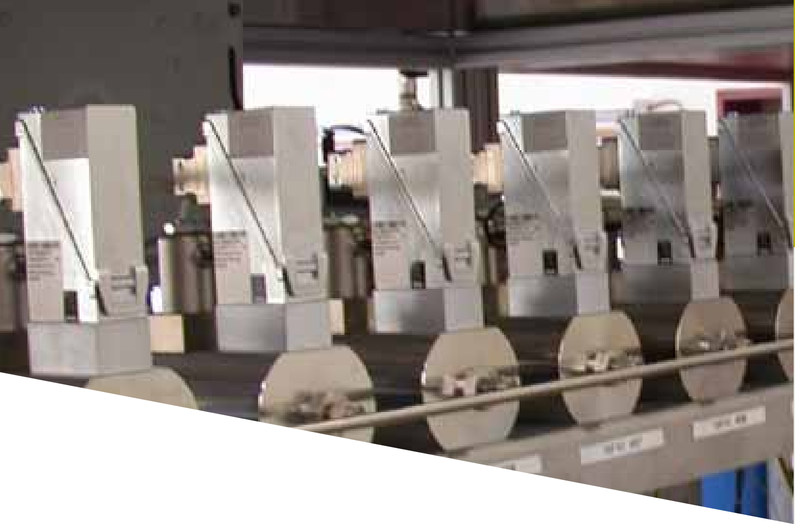
Leverage effect of FISCH
The expectation is that FISCH will provide substantial added value for the further development of the chemical and life sciences industry. Arthur D. Little assessed the potential impact of FISCH on chemistry in Flanders. The annual economic leverage by 2020 is estimated at € 7.4 billion in supplementary turnover, the creation of 13,000 additional direct jobs, and € 300 million in new R&D investment. FISCH will also have positive spill-over effects that are less easy to quantify, such as:

- Creating a more positive environment for innovation
- The growth of new innovation-oriented small and medium-sized enterprises and service companies
- The strengthening of companies through international, multidisciplinary and multisector cooperation agreements
- The development of training courses focused on sustainable chemistry.

Frans Dieryck
Managing Director essenscia vlaanderen

INDEX RESEARCH GROUPS

Competences at the Vrije Universiteit Brussel, related to the FISCH research themes:



Chemical Engineering – CHIS

Vrije Universiteit Brussel
Faculty of Engineering

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Biomass conversion – Separation technology – Microtechnology – Catalysis and alternative energy input – Multifactorial high-throughput methodologies

Research orientations

Biomass conversion

- Cleaning of biomass gasification gas via integrated filtration and catalytic removal of tar components using catalytic candle filters
- Process modeling of biomass gasification processes

Separation technology

The Department of Chemical Engineering has a longstanding tradition in the field of separation technology. In this branch the department takes a unique and leading position among the different research groups in Flanders. CHIS is currently conducting both fundamental and applied research on two key separation technologies: adsorption and chromatography. This research addresses all scales, ranging from the investigation of the processes at the molecular scale all the way up to the development of industrial scale production processes, always combining theory and experiment and putting a large emphasis on process modeling and simulation. Research activities:

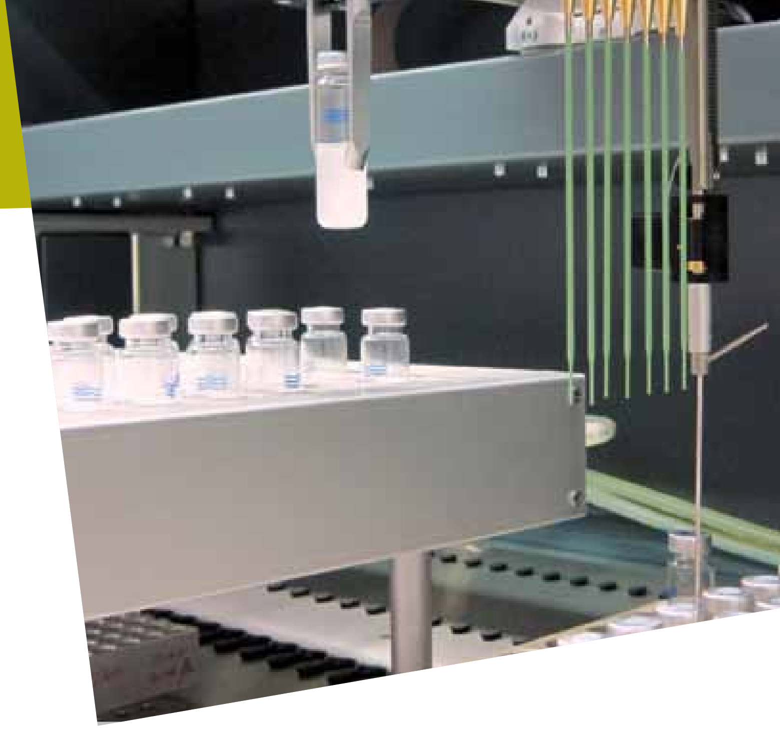
- Separation and purification processes
- Development of liquid chromatography separations in micro-fabricated HPLC columns
- Testing and development of adsorbents for CO_2 capture and separation (synthesis gas, flue gas, natural gas)
- Hot gas cleaning
- Design and modeling of separation and reaction processes (mass and heat transfer, multicomponent adsorption equilibria, dynamic processes, Computational Fluid Dynamics, scale-up,...)
- Metal organic frameworks, hybrid carbon silica materials, zeolites, biporous solids,...
- Solvent purification
- High-throughput testing
- Fabrication and testing of nano-separation devices
- Structured separation devices, monolithic adsorption columns, porous-shell pillar array columns for high resolution liquid chromatography separations
- Ultra-rapid separations of bio-molecules in nano-channels
- Coupling of micro-reactors and separation

Microtechnology

The Department of Chemical Engineering was one of Flanders' pioneers in the microfluidics field and has acquired a vast amount of know-how in the design and the fabrication of microfluidic systems.

Current and new developments:

- Chip design and fabrication (in both silicon and glass, Bosch etching, deep-UV and nano-imprint lithography)
- Microreactors
- Numerical modeling and design of microfluidic systems
- Connection of chips to the outer world (sample injectors, off-chip detectors)
- On-chip separation strategies (chromatography, size fractionation, DNA hybridizations, extraction, membrane separation)
- Optical detection (both on-chip and off-chip, and both fluorescence and UV-Vis absorption)
- Large scale production via replication in plastics (hot embossing)
- Fast prototyping of microfluidic demonstrators
- Design and modeling of fuel cells
- Catalytic reactions between immiscible phases
- Integration into micro-reactors and microfluidic devices
- High efficiency cooling and heating in silicon based reactors
- High-throughput screening for reaction conditions, solvent compatibility,...
- Integrated process analytical technology devices



Catalysis and alternative energy input – heterogeneous catalysis

Within the field of heterogeneous catalysis, relationships between catalyst adsorption properties and catalytic performance are studied at the Department of Chemical Engineering, in close collaboration with other strong groups in Flanders.

Expertise:

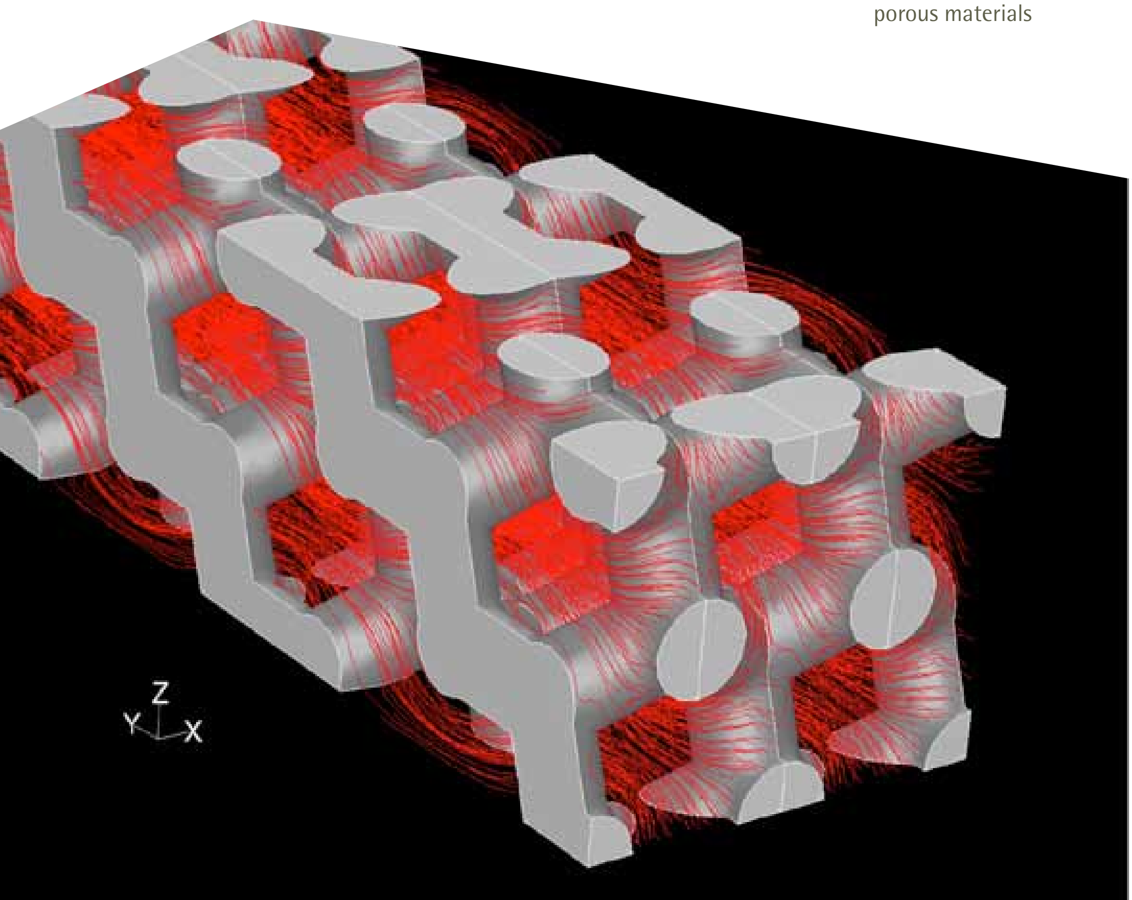
- Modeling of heterogeneously catalyzed reactions using diffusion/adsorption/reaction models
- High-throughput testing of heterogeneous catalysts
- Integration of separation and catalytic processes
- Structured catalytic reactors
- High temperature catalytic cleaning of gasification gas using a catalytic filter
- Adsorption effects in hydrocarbon conversion using zeolites (e.g. Friedel-Crafts alkylations and acylations, catalytic upgrading of Fisher-Tropsch waxes)
- Experimental determination of adsorption parameters for use in reaction modeling
- Modeling of fuel cells for electrocatalytic cogeneration of bulk chemicals and electricity
- Microdevices/microreactors for catalytic reactions

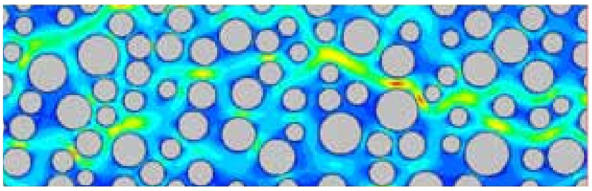
Multifactorial high-throughput methodologies

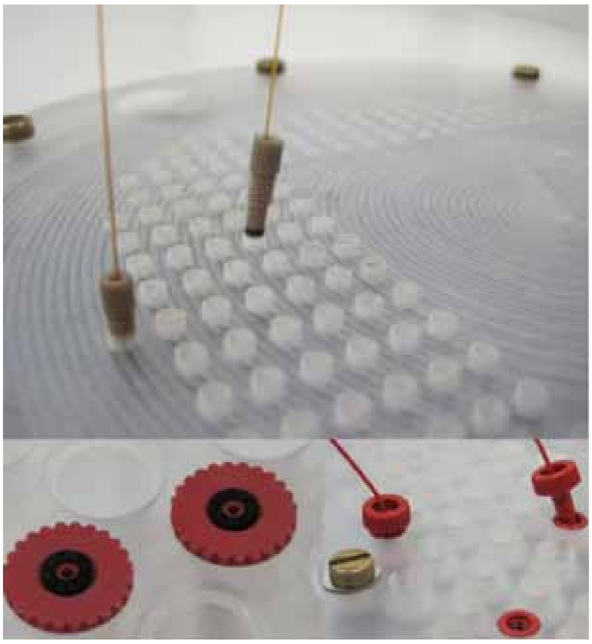
The Department of Chemical Engineering is developing and using high-throughput experimental techniques and devices to screen and evaluate adsorbents and catalysts for industrial applications.

The following expertise is currently available:

- Parallel high-throughput testing of adsorbents and industrial catalysts
- Statistical analysis and numerical modeling of high-throughput experimental data
- Use of high-throughput methods and modeling techniques to optimize chemical processes
- Statistical tools to analyze structure-selectivity relationships in multicomponent adsorption equilibria on porous materials







Equipment & Infrastructure

The Department of Chemical Engineering develops high-throughput devices to characterize and test materials in automated and parallel manner. This equipment allows screening a large number of materials, components and operational conditions. This equipment is unique, worldwide. A wide variety of characterization techniques and analytical instruments is available. Equipment to develop and test microfluidic devices is present.

- Experimental high temperature set-up for testing of catalysts and catalytic filters for cleaning of gases at high temperature
- Fully automated high-throughput device for frontal analysis allowing to measure on 20 adsorption/reaction columns without user intervention: liquid phase, 20-400°C, 1-200 bar, in situ activation, online analysis, fraction collection
- Robotic devices to measure liquid phase adsorption isotherms
- Parallel reaction/adsorption system with 10 reaction/adsorption beds
- 8-channel volumetric device to determine high-pressure gas phase isotherms
- High-throughput set-up for gas and vapor phase breakthrough separation experiments
- Nitrogen and mercury porosimetry
- Pycnometry
- High pressure/temperature gravimetric set-up for pure component isotherms
- Gravimetric/volumetric set-up for multicomponent gas adsorption
- Gravimetric device for vapor adsorption
- GC-MS, GC, MS, HPLC
- Fluorescence microscopes equipped with CCD camera and excitation lasers (3)
- 100-node computer cluster
- Micro-miling robot to produce micro-precision mechanical parts
- Nano- and microflow HPLC system (Ultimate, Dionex) with 2 nl UV detection cell
- On-chip UV-Vis detection set-up
- Reactor set-up for high temperature cleaning of gasification gas
- High-throughput volumetric set-up for measuring isotherms of gases (CO_2, CH_4, H_2, C_2H_6, C_3H_8, ...) on 8 samples

Average capacity of group: 35 persons

Collaboration with industrial partners

Institut Français du Pétrole, Eni, Dow Chemicals, Proviron, UCB, Solvay, BASF, INEOS, TOTAL, Taminco, ExxonMobil, Janssen Pharmaceuticals, Pall Schumacher, Atlas Copco, Agilent, Thermo Scientific, Keppel Seghers, P&G, Umicore

Physical Chemistry and Polymer Science - FYSC

Vrije Universiteit Brussel
Faculty of Engineering

www.vub.ac.be/FYSC

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Sustainable chemical products - Green solvents - Microtechnology - Catalysis and alternative energy input - Separation technology

Research orientations

The research activities of the research group Physical Chemistry and Polymer Science are focused on **molecular and supramolecular structure-processing-property relations** in synthetic, bio-based or natural polymers for developing sustainable materials with improved performance. A unique collection of physicochemical analytical techniques and characterization procedures is available for this purpose. Novel macromolecular materials are designed by polymer synthesis, either in-house or in collaboration with external partners.

A contribution to the international progress of thermal analysis for materials' characterization is aimed at, extending the instrument range to:

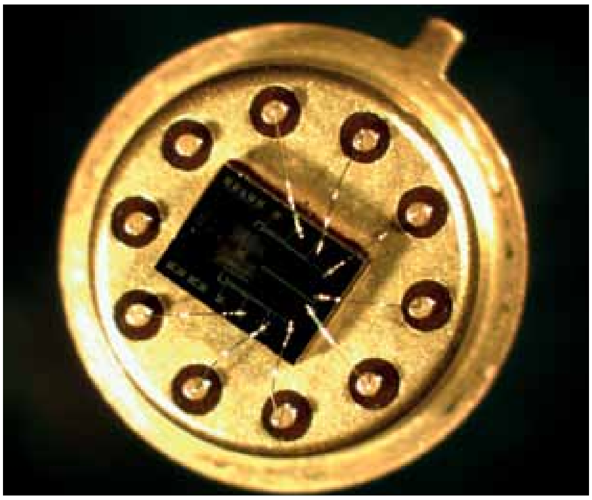
- Techniques for measuring transitions more sensitively: modulated temperature differential scanning calorimetry, micro- and nanocalorimetry
- Faster techniques suitable for thin films and ultra-small samples: ultra fast scanning chip-based methods
- Techniques permitting analyses on a smaller lateral scale: spatially localized thermal analysis at the micro- and nanometer level using atomic force microscopy based methods
- Novel in-house developed hyphenated thermal techniques permitting combinations of measurements on a single sample

Education and training in thermal analysis for the academic and industrial community is also an objective.

Current research projects in collaboration with academic and industrial partners are dealing with:

- Water-soluble and bio(degradable) polymers
- Geopolymers: cement replacement with low carbon footprint
- Self-healing coatings and recyclable thermosets based on reversible physical and covalent polymer networks,
- Polymer: fullerene nanostructured blends for bulk heterojunction solar cells
- Nanostructured polymers and polymer interphases including block copolymers for the aqueous dispersion of nanoparticles, nanocomposites for biomedical applications, smart polymer surfaces, conductive coatings
- Polymer nanofibres that can be used for ultra-filtration
- Stimuli-responsive polymers: thermo- and pH responsive polymers and hydrogels, self-healing polymers

In these materials, we study molecular structure and thermal properties, very slow to very fast reaction and crystallization processes, reaction mechanisms and kinetics, chemorheology, reaction- or crystallization-induced nanostructure formation, stability, degradation, and flame retardance, all supported by predictive modelling.



Current and new activities are directed to:

- Novel trends in polymer science and technology, i.e. nanostructured (hybrid) polymers and supramolecular organisation in polymers and (aqueous) polymer solutions, aiming at more sustainable materials through a judicious selection of building blocks, improving the lifetime of materials, reducing material needs through property enhancement
- A further extension of the thermo-analytical infrastructure with specialized equipment of ultimate performance to allow nanoscale thermal analysis both in the bulk and at the surface of polymer systems
- A continued collaboration with other research teams, bringing together expertise in polymer synthesis, characterization, theory, predictive modelling, and processing

Equipment & Infrastructure

The research group of Physical Chemistry and Polymer Science has a unique infrastructure of thermal analysis equipment in combination with complementary techniques for the physical-chemical characterization of polymer systems:

Measuring thermal properties and transformations

Bulk samples – from milligram to gram scale

- Differential scanning calorimetry (DSC) and modulated temperature differential scanning calorimetry (MTDSC) using Tzero technology
- Multi-channel micro- and nanocalorimetry for isothermal and scanning modes over an extended temperature range, with isothermal titration calorimetry option
- Photocalorimetry for UV or visible light photopolymerizations
- RheoDSC, for simultaneous rheological and calorimetric analysis
- Dynamic rheometry and dynamic mechanical analysis (DMA)
- Thermomechanical analysis (TMA)
- Thermogravimetric analysis (TGA)

Thin films – down to 10 nm

Ultra-small samples – from microgram to nanogram scale

- Rapid heat-cool differential scanning calorimetry – up to 2000 °C/min
- Ultrafast scanning chip calorimetry for studying thin films and nanogram samples at up to 1 000 000 °C/s in heating and cooling
- AC chip calorimetry for studying thin films and nanogram samples
- Hot-stage atomic force microscopy with micro- and nanothermal analysis options for localised thermal analyses down to a 100 nm scale, equipped with a heat-cool stage

Supporting techniques

- Gel permeation chromatography with triple detection suitable for characterizing polymers with complex architectures
- High-resolution ultrasound spectroscopy
- Infrared spectroscopy, with HATR and specular reflectance, and Raman spectroscopy
- NMR spectroscopy, including HR-MAS NMR, relaxation and diffusion NMR, and an extensive range of surface and electrochemical analysis instrumentation are available within the Department for Materials and Chemistry (MACH-VUB) where FYSC is part of

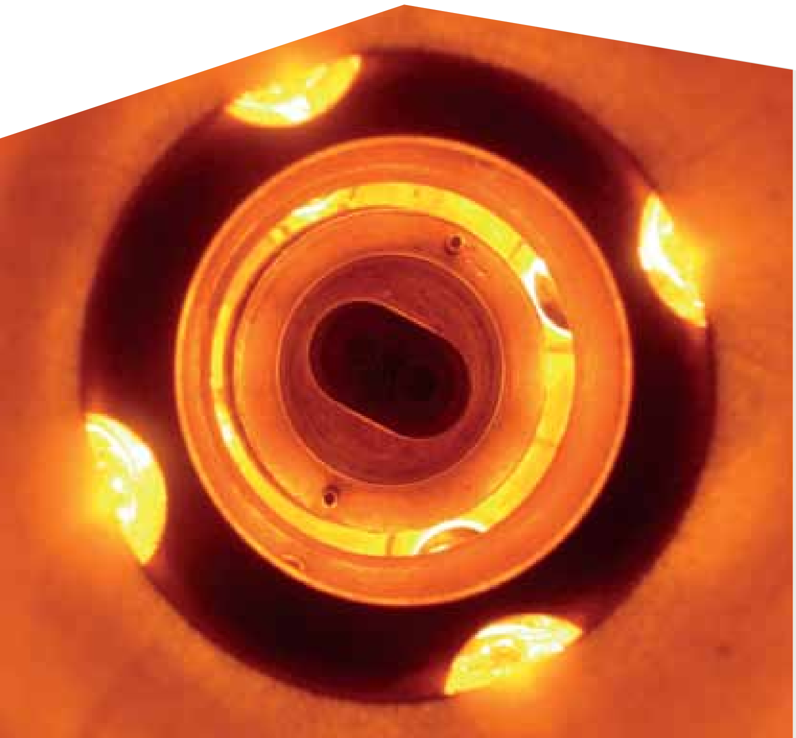
Modelling

- Finite element modelling software permitting the simulation of coupled multiphysics problems, including specialized modules for heat transfer, chemical reaction engineering, and parameter optimization

Average capacity of group: 17 people

Collaboration with industrial partners

AGFA, Bekaert, Centexbel, Cargill-Cerestar R&D, CYTEC Surface Specialties, DSM Research, EXXON Chemical, FINA Research, Huntsman, Milliken, Procter & Gamble, Recticel, Robert Bosch Productions, Rf-Technologies, Shell Research, Solvay



Industrial Microbiology and Food Biotechnology – IMDO

Vrije Universiteit Brussel
Faculty of Sciences and Bioengineering Sciences

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Biomass conversion – Valorisation of side and waste streams – Sustainable chemical products

Research orientations

The research group Industrial Microbiology and Food Biotechnology (IMDO) has the necessary expertise and infrastructure to perform:

Biomass conversion

- White biotechnology, production of platform chemicals and fine chemicals from biomass via fermentation and bioconversion, production of biofuels from biomass

Valorisation of side and waste streams

- Fermentation and bioconversion of substrates from side and waste streams into diverse chemicals and high-performance materials

Sustainable chemical products

- Production of biobased building blocks and biodegradable chemicals and materials from sustainable agricultural raw materials through fermentation and bioconversion

Multidisciplinary research and collaboration initiatives can be set up between the research group IMDO and research groups in applied biological sciences and chemical engineering, so that the complete value chain can be covered from the basic raw materials over optimal fermentation and bioconversion processes to the final sustainable products.

Specific, available expertise and current activities

The following expertise is currently available:

Production of fine chemicals and enzymes for industrial application, consisting of fermentative production processes and their downstream processing, as well as *in situ* production processes using functional starter cultures.

Specific expertise includes:

- Multiphasic analysis of microbial ecosystems, consisting of culture-dependent and culture-independent techniques (PCR-DGGE, real-time PCR), and state-of-the-art metabolite analysis methodologies (metabolite target analysis and metabolic fingerprinting)
- Temporal metagenomic, metatranscriptomic, and metametabolomic analysis of microbial ecosystems
- Genomic and physiological screening of microbial isolates for interesting functionalities
- Functionality-based, metabolomics-based, and genomics-driven fermentation studies in computer-controlled bioreactors
- Kinetic analysis and mathematical modeling of microbial behavior (growth, population dynamics, metabolite production kinetics)
- Elucidation of metabolic pathways involved in functionalities of microorganisms
- Optimization of fermentation and bioconversion processes regarding functionalities of microorganisms
- Evaluation of functionalities of microorganisms through proof-of-principle experiments

Current activities

- Kinetic analysis and modeling of microbial processes, with a focus on growth, competitiveness, interactions, process control, substrate conversions, and metabolite production
- Research on healthier, safer, and more attractive food products, via functional microbial metabolites and functional starter cultures
- Unraveling of complex fermented food ecosystem structures with respect to its microbial communities and functional metabolites
- Research on the functional role of microorganisms in the gut and in fermented food ecosystems, as well as the associated microbe-microbe, microbe-food, and metabolite-food interactions

Specific contribution to the FISCH themes "Biomass conversion", "Valorisation of side and waste streams", and "Sustainable chemical products"

- Genotypic and phenotypic screening of microorganisms for their applicability to produce microbial fine chemicals, platform molecules, and biofuels by fermentation using specific substrates
- Omics approach to discover new functionalities of microorganisms regarding the production of enzymes, fine chemicals, platform molecules, and biofuels
- Optimizing fermentation processes: kinetic analysis and modeling of fermentation processes, testing of operation conditions and process control, downstream processing

Equipment & Infrastructure

The equipment of the research groups includes:

- **Computer-controlled fermentors**, among which 15-liter-scale Biostat C-DCU fermentors and 2-liter-scale Biostat B-DCU fermentors with on line mass and gas ($H_2/CO_2/CH_4$) analysis
- **State-of-the-art analysis platform** based on high-performance chromatography [high-performance liquid chromatography (HPLC), high-performance anion exchange chromatography with pulsed amperometric detection (HPAEC-PAD), high-performance anion exchange chromatography with conductivity monitoring under ion suppression (HPAEC-CIS), and gas chromatography (GC)] and/or mass spectrometry (MS) [GC-MS, HPLC-MS/MS, ultra performance liquid chromatography coupled to mass spectrometry (UPLC-MS/MS), and selective ion flow tube mass spectrometry (SIFT-MS)]
- **Equipment for microbiology and molecular biology**, including incubators, freeze drier, stomacher, ball miller, cell disrupter (sonicator), flow cytometer, electrophoresis apparatus (nucleic acids, proteins, DGGEs), (Nanodrop) spectrophotometers, PCR apparatus (without and with temperature gradient), real-time PCR apparatus, centrifuges, and ultrafiltration apparatus

Average capacity of group: 20

Collaboration with industrial partners

Food, chemical, and pharmaceutical industry

Analytical and Environmental Chemistry – ANCH

Vrije Universiteit Brussel
Faculty of Sciences and Bioengineering Sciences

www.vub.ac.be/ANCH

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Micro algae – Separation technology – Microtechnology

Research orientations

The actual research activities of the Analytical and Environmental Chemistry laboratory rest on four domains of expertise, which are interrelated and under continuous development.

The expertise domains are the following:

- Application and use of tracers (stable isotopes)
- Nutrients and biogeochemical cycles
- Metal speciation
- Bio-assays for organic pollutants
- Modeling and algorithm development

These research activities are applied for assessing:

- The status of natural and perturbed aquatic ecosystems such as open oceans, coastal seas, estuaries, rivers and lakes
- The impact of the environment on health
- The impact of packaging on food quality
- Food safety control

Micro algae

In this research, focus goes to the structural and functional study of arsenic methyltransferases for bioremediation. Via genetic engineering these algae and microorganisms are used to remove arsenic from contaminated water and soil via phytovolatilisation as a new strategy to clean up the environment.

Research activities:

- Cloning genes for ArsM homologues from selected soil fungi, algae
- Structure/function study of arsenic methylation by ArsM
- Comparative characterization of ArsM enzymes from selected bacteria, fungi, algae and aquatic plants

Separation technology

Separation and purification processes are used for studying metal speciation, dioxin and dioxin-like compounds:

- HPLC
- GC
- ASE
- Passive sampling devices

Microtechnology

Development of sensitive micro-electrodes based on nanotechnology.

Current and new developments

- Development and validation of stable isotope techniques applied to nitrogen and carbon studies in aquatic systems
- Development of new passive samplers with new resins for inorganic compounds. They can be used for purification of contaminants in industrial processes or waste water treatment.
- Testing of ceramic tubes for trapping persistent organic pollutants in sediment pore waters
- Development of micro-electrodes based on nanotechnology.
- DRE- and ERE-CALUX bioasays
- Statistics and chemometrics for analytical and environmental chemistry
- Development of models to extract information from measurements using passive sampling devices (DGT and DET)

Equipment & Infrastructure

The department of Analytical and Environmental Chemistry has a wide variety of analytical instruments at its disposal. These include:

- Microscope and haemocytometer
- Nucleocounter
- Luminometer
- QuAAtro nutrient analyser
- UV-VIS spectrophotometer
- Stand metrohm voltammetric devise
- CV-GC-AFS
- LA-ICPMS
- GC-IRMS
- Dionex
- DET/DGT probes

Equipment & infrastructure specifically used in the micro algae domain:

- HR-ICPMS (Thermo Finnigan, Element II) for the determination of total arsenic concentrations
- automated continuous flow hydride generation/atomic fluorescence spectrometer (Excalibur 10.003, PS Analytical) for the determination of hydride forming arsenic compounds.
- HPLC coupled to the HG-AFS for arsenic speciation
- EA-IRMS with Conflo III interface (Thermo Finnigan, DELTA Plus) for the measurements of $\delta^{15}N$ and $\delta^{13}C$ in algae
- elemental analysers for POC and PN measurements
- DIC/DOC Analyser

Average capacity of group: 30

Collaboration with industrial partners and institutions

- Belgian Packaging Institute (BPI)
- Federation of paper and cardboard processing Industry (FETRA)
- Veterinary and Agrochemical Research Centre (CODA-CERVA)
- Belgian Scientific Institute for Public Health (WIV-ISP)
- Belgian Nuclear Research Centre (SCK-CEN)
- Royal Museum for Central Africa(RMCA)
- Brussels Instituut voor Milieubeheer (IBGE-BIM)
- Flemish Institute for Technological Research (VITO)
- AREVA

Organic Chemistry – ORGC

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Catalysis and alternative energy input – Biomass conversion – Fine chemicals from biomass

Research orientations

Homogeneous catalysis

Within the field of homogeneous catalysis, new methods are being developed to synthesize heterocyclic compounds with use in medicinal chemistry and compounds with use in oleo- and polymer chemistry. The research is focused on gold and copper catalyzed alkyne functionalizations, and includes the following topics:

- Synthesis of polyheterocycles via AU(I)- and AU(II)-catalyzed cyclization of alkynated amines and amides
- Gold-catalyzed transformations of 1,3-diynes
- Synthesis of N-heterocycles via Cu-catalyzed transformations of functionalized alkynes and diynes
- The use of Cu-catalyzed diyne coupling in peptide homo- and heterodimers and cyclopeptide chemistry

Visible light induced photoredox catalysis

The new research field of visible light photocatalysis using low energy LED- or power save lamps is being evaluated as a tool to synthesize new carbo- and heterocyclic compounds, including:

- Exploration of new radical cascade reactions, generated via visible light activation of ruthenium catalysts (e.g. Ru(II)(bipy)3), as new methods in heterocyclic chemistry
- Functionalization of alkenes and alkynes via photoredox catalysis (use of blue/red/green LED-lamps as alternative energy sources in photochemistry)

Peptide and peptidomimetic chemistry

The research group of Organic Chemistry has a long standing expertise in the synthesis of bio-active peptides and peptidomimetics. In this research topic, both peptide chemistry as well as heterocyclic chemistry are intensively studied.

- Synthesis of new azepane containing structures as new templates in medicinal chemistry
- Synthesis of spirocyclic azaheterocycles as new building blocks in peptidomimetic chemistry
- Structural analysis of helix- and turn-inducing compounds and application in the synthesis of bio-active peptidomimetics
- Evaluation of helix stabilizing effects for use in the synthesis of new bio-active peptides and peptidomimetics
- Synthesis of peptide-based biopolymers
- Synthesis and biological evaluation of new antimicrobial peptides
- Synthesis of bi- or multifunctional receptor ligands for pain research

Equipment & Infrastructure

At the research group of Organic Chemistry, an extended infrastructure and in-house equipment is available which allows us to cover a broad range of activities in organic synthesis. Standard laboratory infrastructure as well as the following specialized synthesis and analysis equipment is used for own research and for external services, e.g. NMR, HRMS, LC-MS analyses.

- AVANCE 2 Bruker 500 NMR instrument
- AVANCE Bruker DRX 250 instrument
- High resolution LC-MS (HRMS)
- HPLC systems with autosampler and degasser, UV detector and thermostated column compartment with an operating temperature range from ambient to 105° C.
- Semi-preparative HPLC system with 322 pumpmodel, UV detector UV-VIS 156, manual injector and 206 Fraction Collector
- Automated Peptide Synthesizer
- Freeze drying equipment
- UV spectrometer
- IR spectrometer
- Optical Rotation equipment
- Parr hydrogenation equipment (up to 4 bar)
- HF-apparatus connected to a HF-absorption cylinder

Average capacity of group: 20

Collaboration with industrial partners

Janssen Pharmaceutica, Galapagos, Solvay, Recticel, Denys, ...

Structural Biology Brussels – SBB

Vrije Universiteit Brussel
Faculty of Sciences and Bioengineering Sciences

www.structuralbiology.be

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Biocatalysis – Microtechnology

Research orientations

The Structural Biology Brussels (SBB) laboratory is an independent research group supported by VIB (Flanders Institute for Biotechnology).

Biocatalysis

Enzymes are biocatalysts which distinguish themselves in their unique catalytic properties (rate enhancements of up to 10^{17}) and specificities (often even strict enantioselectivity). They commonly achieve these unique properties in a neutral water environment at ambient temperatures (20°C-37°C). These properties make enzymes extremely suitable for **biotransformations** with a **minimum of energy input and without use of organic solvents and other polluting waste streams** (so-called "white biotechnology").

SBB has a strong tradition and expertise in the study of the structure and function of **enzymes and their engineering and design towards new properties and applications**. In this approach enzymes with desired properties can be isolated from natural sources or expressed recombinantly. Afterwards the enzymes can be further engineered toward better selectivity (or even new functions) and other desired properties such as increased stability. In this respect all the knowhow and technology for enzyme engineering is present in the department. More specifically, we have the expertise and equipment to study the biophysical (ITC and DSC calorimetry, UV-VIS spectroscopy and fluorimetry, CD, DLS), kinetic (stopped flow, quenched flow) and structural (X-ray generator, NMR and AFM) properties of proteins and enzymes. And we have a high access to synchrotron facilities.

Nanotechnology

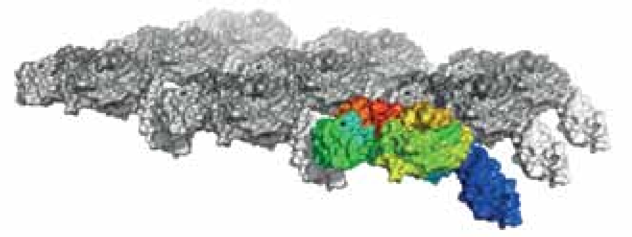
In recent years, the scientific community has gained increased interest for the application of **biological materials** in bottom up approaches for nanotechnology developments. Many biological systems contain self-organizing molecules that condense in ordered networks with functions ranging from molecular motors, switches and pumps to regular 1D and 2D scaffolding materials. These systems contain intrinsic characteristics that could be harnessed for the fabrication of **biosensors, lab-on-chip applications and nanoelectronic devices**.

Part of the ongoing research in the group Structural & Molecular Microbiology, a division of SBB and VIB, looks at the structural organization of **proteinaceous polymers found on bacterial cell surfaces**. These can be found to form regular filamentous or two-dimensional arrays formed of repetitive units assembled in defined conformations. Through the knowledge of the tridimensional structure of the protein building blocks and their mode of assembly inside the polymers, one can come to the rational design of functionalized bottom-up materials such as patterning and display scaffolds for chemical and biological catalysts. When deposited on biological and non-biological surfaces, interfaces and porous membranes, the high density, topologically idealized display of the catalysts provides a tool for process intensification and continuous product separation.

A second emerging topic concerns the **functionalization of organic or anorganic materials** (polymers, membranes, nanoparticles, ...) with **nanobodies**. The occurrence of bona fide antibodies devoid of light chains in Camelidae by Emeritus Prof. Raymond Hamers was one of the major discoveries within our department. Nanobodies are the recombinant minimal-sized intact antigen-binding domains from such camel heavy-chain antibodies. Like conventional antibodies, nanobodies show high target specificity, high affinity for their target end low inherent toxicity. Nanobodies can be expressed efficiently in bacteria as active, soluble, and robust proteins and are amenable to applications beyond therapeutics including applications in material sciences.

Equipment & Infrastructure

- Molecular biology and recombinant DNA technology for protein and enzyme engineering and design
- Protein purification facilities (Äkta low and medium pressure systems, Waters HPLC)
- Biophysical equipment
    - UV/VIS spectrophotometer (3 Varian Cary 100)
    - Fluorimeter (Perkin-Elmer)
    - Isothermal titration calorimetry (ITC) (Microcal)
    - Differential scanning calorimetry (DSC) (Microcal)
    - Circular dichroism (CD) (Jasco)
    - Surface plasmon resonance (Biacore 3000)
    - MicroscaleThermophoresis (Nanotemper)
- Enzyme kinetics
    - Stopped-flow fast kinetics devise (Applied Photophysics)
    - Quenched-flow fast kinetics devise (KinTek)
    - Spectramax 340C (Molecular devices)



- Structural methods
    - X-ray crystallography (Rigaku 007-VHF microfocus rotating anode and 944+ CCD detector)
    - NMR Varian 600MHz and 800 MHz (with cryo-probe)
    - Atomic force microscope (AFM) (Multimode NanoscopeIIIa AFM from Veeco)
    - Confocal laser microscopy (Nikon D-Eclipse C1)
    - Automation
    - Crystallisation robot (Phoenix, Art Robbins)
    - Liquid handling system (Formulator, Formulatrix)
    - Tecan robot system

Average capacity of research group:
6 group leaders, more than 70 researchers and technicians

Collaboration with industrial partners

Galapagos, Ablynx Roche, Novo Nordisk, Cargill

Electrochemical and Surface Engineering – SURF

Vrije Universiteit Brussel
Faculty of Engineering

www.vub.ac.be/SURF

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Green solvents – Microtechnology – Sustainable chemical products

Research orientations

The main research topic of SURF is **surface engineering of metals**, which implies surface characterization and surface treatments in order to obtain specific properties (mechanical, optical, corrosion resistance, etc). In the broad field of surface treatments, SURF has experience in electrodeposition processes, anodisation, conversion treatments, coatings, ...

Corrosion engineering is an important field of expertise of SURF: study of corrosion mechanisms, characterization of protection methods (inhibitors, organic coatings...), corrosion management.

Modelling is more and more involved as tool to optimize production techniques (reactors, printed circuits boards..) and to predict durability of materials (corrosion).

Specific topics

Environmentally sound surface treatments of metals:

- Cr 6+ free surface pre-treatments of aluminium alloys, steel and galvanized steel such as etching, anodizing, silane coating, phosphatation, zirconium-titanium conversion treatments, PVD coating, plasma coating, self-healing coatings etc.

Materials' sustainability and corrosion research

- Study of corrosion mechanisms of aluminium alloys, steel, stainless steel, copper and titanium
- Characterization of corrosion protection of metal alloys by organic coatings for durable performance
- Study, prediction and modelling of corrosion of aluminium alloys for example for aerospace applications

Surface engineering for multifunctional surface properties of metals

- Electrocolouring of anodised aluminium for building applications using environmentally and economically sound technology
- Durable thermal performance of hard anodised lead-free aluminium machining alloys for automotive brake systems
- Organic surface pre-treatments with incorporated nanosize metal oxide particles for multifunctional surface properties of aluminium and steel
- Multiple action self-healing coatings

Electrochemical process engineering

Batteries and fuel cells

- Study of electrode mechanisms
- Characterization of electrode materials by surface analysis
- Impedance measurements

Equipment & Infrastructure

SURF is in the unique position of having an advanced technological infrastructure and electrochemical software/ modeling tools.

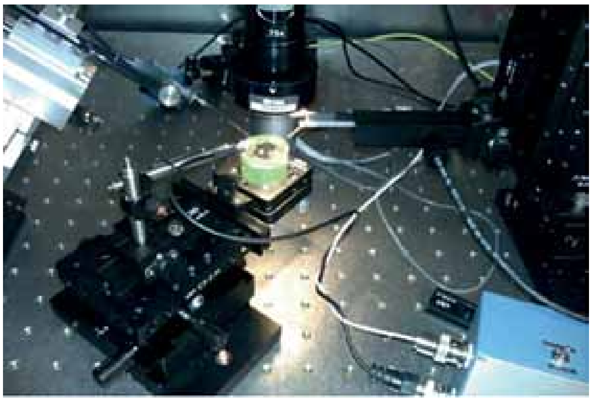
- Complementary electrochemical methods
    - Electrochemical Impedance Spectroscopy Methods
    - Electrochemical Stationary and Non Stationary Methods
    - Electrochemical reactors operating under different flow regimes (e.g. rotating disc reactor, wall jet reactor, parallel flow reactor)

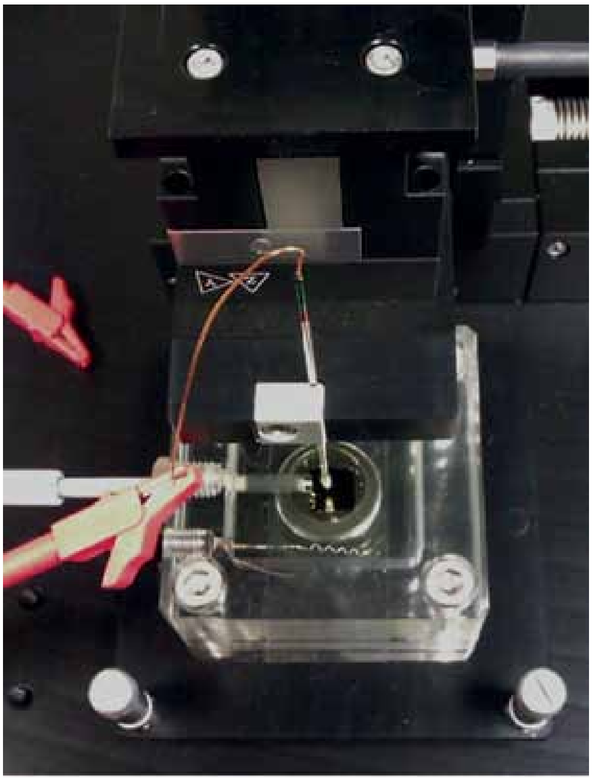
- Local electrochemical methods
  - Scanning Electrochemical Microscopy (SECM)
  - Scanning Vibrating Electrode Technique combined with Scanning Ion selective Electrode Technique (SVET/SIET)
  - Atomic Force Microscopy combined with in-situ electrochemical cell (AFM)
- In-situ and ex-situ surface analytical techniques
  - Scanning electron microscopy (FE-SEM)
  - Auger electron spectroscopy (FE-AES)
  - X-ray photoelectron spectroscopy (XPS)
  - In situ Spectroscopic ellipsometry (visual and infrared)
  - Confocal Raman spectroscopy
  - In situ AFM-STM
- Electrochemical modeling tools
  - Numerical software for macro, meso & micro scale systems
  - Dedicated fitting tools based on maximum likelihood estimator

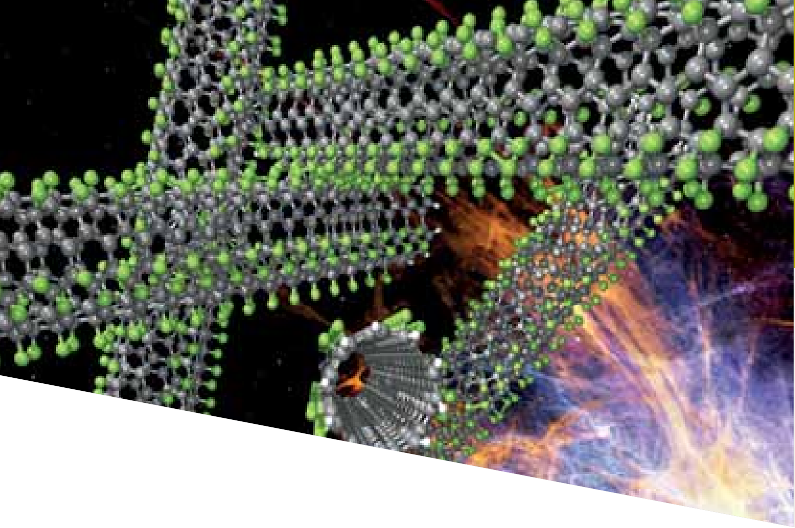
Average capacity of research group: 40 researchers + 9 administrative & technical staff

Equipment & Infrastructure

Afga Gevaert, Aleris, ArcelorMittal/OCAS, Asco, BASF, Bekaert, Bodycote, Chemetall, Coil, Cormet Testing Systems, Corus, EADS/Airbus, Elsyca, FLAMAC, Henkel, Hydro, Infineon Technologies, SEZ AG (division of Lam Research Corporation), Technikon, Umicore, AtlasCopco, EMAX







General Chemistry – ALGC

Vrije Universiteit Brussel
Faculty of Sciences and Bioengineering Sciences

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Separation Technology – Catalysis and alternative energy input – Microtechnology – Sustainable chemical products

Research orientations

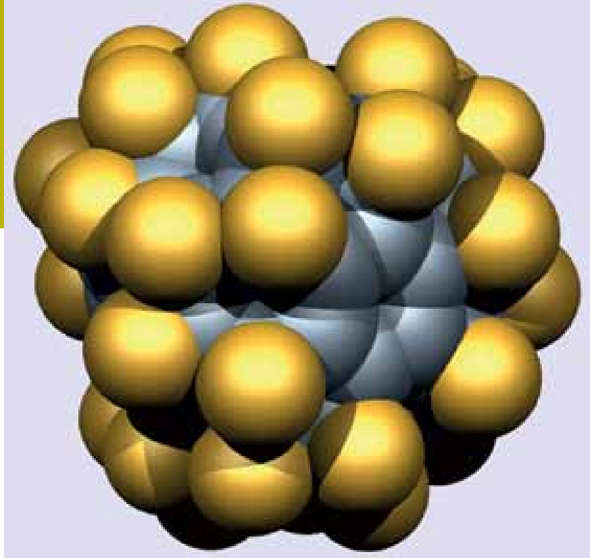
In recent years the interplay between theory and experiment has become crucial in many areas of chemical research and development. Important advances in computational techniques now allow modelling large-scale systems in real-life situations. In particular, Quantum Chemistry (i.e. the application of quantum mechanics to chemical problems such as structure, stability and properties of molecules and their behaviour during reactions) has made enormous progress via the so-called Density Functional Theory (DFT). The main research of ALGC focuses both on the development of concepts as on the application of DFT for specific chemical problems (conceptual and computational DFT).
Fundamental research is performed on the development of DFT-based molecular charge distribution and reactivity descriptors and on the development and testing of related concepts. Applications are considered in organic and inorganic chemistry, in catalysis, biochemistry and materials chemistry, including both kinetic and thermodynamic aspects. Reactions in gas phase, solution and on surfaces are studied. Substrates and topics studied include catalytic and adsorption properties of zeolites, adsorption on silver surfaces, electronic and mechanical properties of fullerenes, carbon nanotubes and graphene, properties of organic functional groups and the reactivity of radicals, in direct interaction with experimental research groups and industry.

Separation Technology

Microporous materials like e.g. zeolites are often used in separation of various mixtures. In the past, our calculations have been used as guidelines to investigate the adsorption behaviour of different molecules in zeolites with different frameworks in order to predict quantities like Henry constants and heats of adsorption.

Catalysis and alternative energy input

Heterogeneous catalysis is of very great importance to the chemical industry. The rather complex reaction mechanisms associated to many of these transformations create a challenging problem for computational chemistry, affording an important synergy between experimental work and theoretical modelling. Our research group has been active in the detailed scrutiny of different catalytic processes, focusing mainly on the use of reactivity descriptors for explaining trends observed in the activities of different catalysts. Previously, we investigated zeolitic materials focusing both on zeolite acidity and basicity. Recently, attention was devoted to supported **vanadium** and **molybdenum oxides**. These materials catalyse a variety of important reactions like the selective oxidation of alkanes and alkenes or the oxidation of o-xylene to phtalic anhydride. For these materials, it was found that the oxide support dramatically influences the rate of the reaction, which was explained by invoking chemical concepts computed for the catalyst. In the initial phases of our work, the catalyst was modelled by a small molecular cluster, but the group has now extended its focus towards a more realistic modelling of the material using periodic calculations.



Microtechnology

Carbon nanotubes recently found application for the development of low-cost sensing elements and low-power consumption gas sensors. **Chemical gas sensors** have now been developed with an active layer of multi-walled carbon nanotubes with chemical functionalisation performed using RF-Plasma under different reaction conditions and plasma composition (oxygen, ferrocene, acrylic acid).

Our calculations allowed to predict the different adsorption properties of **hazardous gases** and the interaction of gas molecules with carbon nanotubes. The presence of functionalised defect sites after plasma treatment and their interaction with gas molecules was demonstrated, showing the power of theoretical research for the development of gas sensing devices by predicting the reaction mechanisms for gas detection and the effect of chemical functionalisation to differentiate the sensor responses.

Sustainable chemical products

One of the most important aims of nanotechnology today is the development of new **composite materials**. Hereby the high need for sustainable products results in important technological challenges concerning their intrinsic properties, their cost, their processing and fabrication, and their ability to be recycled or reused efficiently. Besides mechanical reinforcement of such materials, applications range from daily life to high-end technology in the electronic, automotive, aeronautic and aerospace industry.

Owing to their extraordinary intrinsic properties, carbon systems offer great potential as nanofillers for the production of nanostructured composite materials. Functionalised **fullerenes** are applied for organo-photovoltaics, and due to their high aspect ratio and excellent mechanical and electronic properties, **carbon nanotubes** and **graphene** can provide a three-dimensional network trough the polymer with very low percolation thresholds, resulting in low weight polymer-based composite with significantly improved mechanical and/or electronic properties.

Current research topics include the analysis of fullerenes for the development of **next-generation solar cells**, and of carbon nanotubes and graphene for **mechanical reinforcement** of nanocomposites and **high-end electronic applications**. Our research group has extensive expertise in the theoretical modelling of carbon nanostructures for the development of nanocomposite materials. Analysis of the intrinsic properties of the nanofillers and interaction with polymer matrices has allowed to accurately predict the properties of the nanofillers and the resulting materials by **multidisciplinary** and **multi-scale approaches** in order to assist the experimental synthesis of nanocomposites.

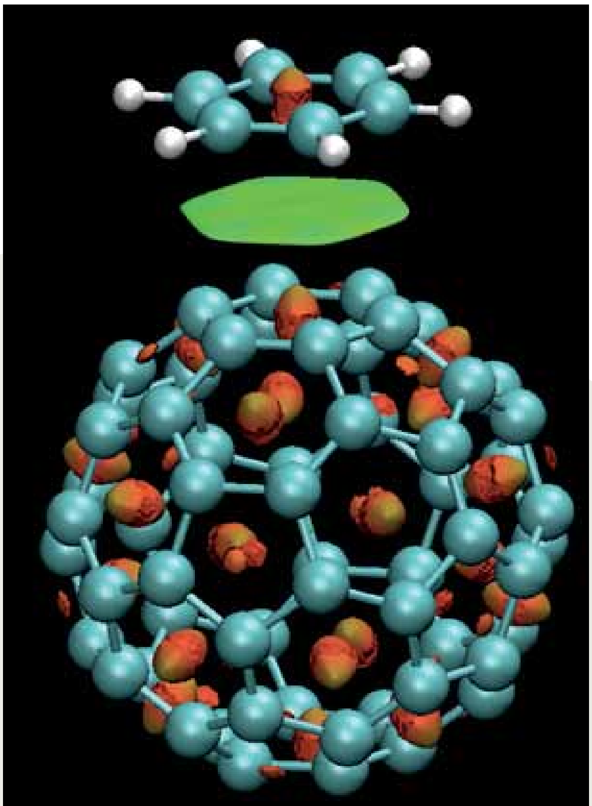
Equipment & Infrastructure

- Modellisation of chemical reactions in various conditions (gas phase, solution, surfaces), using a variety of software packages (Gaussian09, SIESTA, VASP, etc.)
- Hardware equipment: local and external computer configurations, including dedicated computation nodes at the HYDRA configuration of the VUB/ULB Computing Centre (http://new-hydra.vub.ac.be/)

Average capacity of group: 20 persons

Collaboration with industrial partners

Solvay, ExxonMobil, Janssen Pharmaceutica, Mallinckrodt



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