



INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS OF THE CAS, v. v. i.

Research Strategy Plan of ICPF for 2023-2027



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Our Mission:

The Institute of Chemical Process Fundamentals of the CAS strives to advance the chemical and biochemical industries through the development and application of engineering solutions, environmental engineering, and materials science research. We aim to enhance the fundamental understanding of these processes and transfer basic research findings into practical applications and technologies.

Our Vision:

Our vision is to be a leading institution in the development of innovative engineering solutions, sustainable environmental technologies, and advanced materials, contributing to the betterment of society and the environment.

Our Values:

We are committed to excellence in research, education, and innovation, as well as ethical and responsible conduct in all our activities. We foster a collaborative, diverse, and inclusive environment that values creativity, curiosity, and critical thinking. We are dedicated to communicating our research findings to the scientific community and the general public and to contributing to the development of a sustainable future.

Strategic Research Plan:

The Institute's strategic research plan is structured around three core areas: Chemical Engineering, Environmental Engineering, and New Materials. We will foster cross-disciplinary collaborations to address grand challenges in the following focus areas:

Chemical Engineering: The department focuses on fundamental understanding and developing innovative engineering solutions to the challenges faced by the chemical and biochemical industries. Our research will concentrate on the areas of multiphase hydrodynamics, membrane separations, heterogeneous catalysis, and microbial technology. We will employ targeted experiments and multiscale modelling, ranging from particle-based simulations of confined fluids, energetic materials, and granular media to computational fluid dynamics (CFD) of microfluidics.

Environmental Engineering: The department combines two research groups to tackle environmental challenges and advance sustainable solutions. We focus on Aerosols Chemistry and Physics, studying airborne particles' characteristics, composition, and interactions with clouds and trace gases. Additionally, we investigate Waste Management and Sustainable Technologies, developing methods for treating and recovering municipal and industrial waste. Our interdisciplinary research aims to create a better future through practical environmental solutions.

New Materials: The department specializes in the development and application of advanced materials across various fields, including biomedical research, inorganic materials, and organic/hybrid materials. Our research groups focus on key areas such as hydrogen fuel cells, efficient water electrochemical splitting, and flow organic redox batteries. Through collaboration with industry partners, we aim to transfer our findings into practical applications and contribute to the advancement of materials science for a sustainable future.

Overall, our strategic research plan will be aligned with our mission, vision, and values, and will emphasize excellence, innovation, sustainability, and collaboration.



Department of Chemical Engineering

The Department of Chemical Engineering endeavors to apply engineering solutions to current challenges in the chemical and biochemical industries while also enhancing the fundamental understanding of these processes. The research groups work together closely to transfer basic research findings into practical applications and technologies. Although each group has a distinct focus, they strive to advance knowledge in various areas, including multiphase hydrodynamics, membrane separations, heterogeneous catalysis, and microbial technology. To achieve this, they employ targeted experiments and multiscale modelling, ranging from particle-based simulations of confined fluids, energetic materials, and granular media to computational fluid dynamics (CFD) of microfluidics.

Team name: [Research Group of Membrane Separations](#) | **Team Leader:** Petr Stanovský

Our team's vision aims to push the boundaries of membrane-based separations for both gas and liquid mixtures. Our research in the field of gas separation focuses on improving polymeric membranes for more efficient separation of greenhouse gases such as CO₂ or volatile organic compounds. We plan to achieve this through the development of new membranes employing the synergy of task-specified ionic liquids and functional additives like metal-organic frameworks and 2D materials. The team's research activity involves analyzing membrane behavior in a wide range of operational conditions, from CO₂ lean waste gas mixtures to more concentrated streams like raw biogas, including the removal of minor pollutants such as H₂S and SO₂. In liquid-based separations, the team aims to improve the resolution of enantiomers using a suitable chiral selector combined with ionic liquids to increase chiral selectivity and by incorporating functional particles controlled by external fields, such as magnetic or electric fields, to enhance separation efficiency. For both directions, we will combine molecular and numerical modelling for effective pre-selection of membrane materials, chiral selectors, and membrane process optimization.

Team name: [Research Group of Catalysis and Reaction Engineering](#) | **Team Leader:** Karel Soukup

Our team's vision aims to enhance the knowledge in heterogeneous catalysis engineering through developing catalysts, designing catalytic reactors, and determining phenomenological kinetics. Special emphasis is placed on the development of new catalysts and catalyst supports targeted for industrial applications for responsible care production (e.g. Guerbet coupling of bioethanol and biobutanol or hydrogen sulfide direct catalytic decomposition as a refinery waste product). The team believes that besides catalysts and sorbents with complex hierarchical properties, the polymeric nanofibrous catalysts prepared by the electrospinning technique can be a new class of catalysts that will find practical applications in various fields (e.g. in air protection by catalytic total oxidation of volatile organic compounds). Last but not least, the team will use the most current gas sorption models based on Density Function Theory to perform the advanced texture analysis of catalysts and sorbents.

Team name: [Research Group of Multiphase Reactors](#) | **Team leader:** Maria Zedníková

Our team's vision is to enhance the fundamental understanding of the transport phenomena in multiphase systems at different temporal and spatial scales. We systematically study bubbly flows, granular flows, and suspension flows to understand the relation between interactions of individual objects (bubbles/drops/particles) and the macroscopic behavior of multiphase systems. Our first aim is to investigate the dynamic changes of bubbles and microbubbles in various situations (bubble formation, stability, coalescence, and breakup) and their impact on macroscopic behavior in bubble columns and other bubbly systems. We also aim to understand the adsorption mechanism of various



compounds (ions, surfactants, and nanoparticles) at the bubble interface and their consequences on hydrodynamics and mass transfer in bubbly flows and thin liquid films. We strive to develop theoretical models that describe the dynamic behavior of powders and granular materials characterized by various particle sizes, shapes, and material properties (investigating both dry granular and wet suspension flows). Additionally, we investigate the rheology of complex fluids and dispersions for possible enhancement of heat transfer ability and other applications.

Team name: [Research Group of Molecular and Mesoscopic Modelling](#) | **Team leader:** Martin Lísal

Our team's vision is to advance the fundamental understanding of the macroscopic behavior of matter from a microscopic perspective. Our focus is on confined fluids in and out-of-equilibrium relevant to nanofluidics, heterogeneous systems at high-T and high-P relevant to energetic materials, and mechanics of fluid-saturated granular media relevant for energy storage and recovery applications. To achieve this, our research group employs a range of simulation and statistical mechanics techniques as complementary tools to experiments.

Team name: [Research Group of Algal and Microbial Biotechnology](#) | **Team leader:** Irena Brányíková

Our team's vision is to advance the field of microalgal biotechnology by exploring and utilizing the potential of microalgae in food and feed production, organic agriculture, carbon storage and utilization, and other environmental applications. Our goal is to contribute to a sustainable and environmentally friendly future by utilizing microalgal biotechnology in various fields. We will focus especially on developing and implementing technology (i) to capture carbon dioxide from food-grade waste sources, such as fermentation of gases, while simultaneously producing microalgal biomass suitable for nutritional purposes, (ii) to utilize fresh (non-dried) microalgal biomass in human nutrition to reduce costs and improve the quality of food supplements, (iii) to bioremediate eutrophic and hypertrophic waters by intentionally cultivating algae in an innovative floating photobioreactor, (iv) to utilize microalgae in organic agriculture to form a biostimulant preparation.

Team name: [Research Group of Microreactors](#) | **Team leader:** Petr Stavárek

Our team's vision is to use microreactors as intensification tools to increase efficiency, and safety, and reduce the environmental impact of chemical processes. We focus on designing, prototyping, and experimental validation of microreactors for specific applications. Our approach is based on a deep understanding of reaction and transport phenomena to identify the rate-limiting steps and design a tailor-made solution for industrially relevant case studies.

In particular, we focus on three specific topics. First, highly functional, cold-plasma-modified, thin films based on $g\text{-C}_3\text{N}_4$ for visible-light-induced pollutant degradation and water splitting in microreactors. Secondly, batch-to-continuous synthesis transformations using microreactors in pharma and fine chemical industry: phase-transfer catalyzed *N*-alkylation. Thirdly, exploitation of additive manufacturing technologies for (micro)reactor and catalyst support design: optimization of two-phase flow hydrodynamic and transport characteristics of 3D structures as catalyst support in trickle bed reactors.



Department of Environmental Engineering

This Department consists of two research groups: **Aerosols Chemistry and Physics** and **Waste Management and Sustainable Technologies**.

Aerosols Chemistry and Physics group studies liquid and solid particles in the air, their number and mass concentration, chemical composition, and the interaction of these particles with forming clouds and reactive trace gases present in the ambient air. These studies are motivated by changing climate, water cycle, and adverse health effects caused by inhaled aerosols.

The group of **Waste Management and Sustainable Technologies** leads investigations in the field of waste management, recycling, and sustainable technologies with regard to the circular economy. They aim to develop methods for the treatment/recovery of various municipal and industrial wastes and waste materials.

Team name: [Research Group of Aerosols Chemistry and Physics](#) | **Team leader:** Vladimír Ždímal

The research group of **Aerosols Chemistry and Physics** focuses on better understanding the behavior of atmospheric aerosols. Our main focus is on particle size distributions since particle size is a key parameter. The other key topic is the chemical composition of aerosol particles. For example, both a particle's size and its chemical composition determine whether the particle will serve as cloud condensation nuclei, therefore driving the indirect effect of aerosols on climate. Hygroscopicity, which is dependent on both particle size and chemical composition, influences which part of the human respiratory tract particles will deposit, with chemical composition later driving the body's response. Aerosol hygroscopicity and resulting particle size influence visibility through the aerosol. In addition to that, the chemical composition of aerosols based on concentrations of marker compounds, together with a particle size distribution, can serve as a basis for detailed source apportionment/receptor modeling. The research group also contributes to the European Research Infrastructure Consortium ACTRIS providing a calibration laboratory for aerosol spectrometers and counters. Occupational exposure to aerosol (nano) particles will be studied in the research group since it was shown to lead to elevated levels of specific biomarkers in the body fluids of workers. The interaction of aerosol indoors with cultural artifacts will also be studied including advanced techniques for restoration of library and archival collections using aerosol technology.

Team Name: [Research Group of Waste Management and Sustainable Technologies](#) | **Team leader:** Michal Šyc

Our team's vision is to advance the field of waste management, recycling, and sustainable technologies with regard to the circular economy. We aim to develop innovative methods for the treatment and recovery of various municipal and industrial wastes. A particular area of interest is the treatment of fly ash from waste incineration to remove hazardous properties and exploit recovery potential. We will also focus on metal-bearing wastes, such as WEEE and mine tailings. Through the application of mineral processing and hydro/pyrometallurgical methods, we aim to extract and up-concentrate valuable metals from these waste materials. Our focus will also be on verifying the effectiveness of the LARCODEMS separator for separating various plastics and metals from granular mixtures. To support our research and decision-making processes, we will evaluate various wastes using techniques such as material flow analysis and statistical entropy. This approach will enable us to better understand the composition of different waste streams, assess their recovery potential, and identify any environmental concerns associated with their treatment. In addition, we will develop methods for the capture of pollutants, mainly mercury, and greenhouse gases, from flue gases for solid fuel incineration.



Department of New Materials

The Department of New Materials seeks to progress the development of advanced materials in various fields, including biomedical and biomaterial research, inorganic materials, and organic and hybrid materials. Each research group has its specific focus, but all aim to make significant contributions to the field of materials science through the development and application of novel materials and techniques.

Team name: [Research Group of Laser Chemistry](#) | **Team leader:** Radek Fajgar

Our team's vision is to lead the way in the development of novel inorganic materials using advanced methods such as laser/radiofrequency/CVD techniques and chemical vapor deposition. We will thoroughly characterize the materials and explore their application potential, with a focus on the development of efficient catalysts for electrochemical CO₂ reduction to produce valuable fuels such as methanol, ethanol, and organic acids. We will also explore nanostructured catalysts based on metals, such as Pt and Pt/Fe, for use in hydrogen fuel cells. In addition, we aim to scrutinize anodic materials based on thin layers, such as Ni, Ni/Fe, and Pt/IrO_x, to improve the efficiency of water electrochemical splitting.

Team name: [Research Group of Advanced Materials and Organic Synthesis](#) | **Team leader:** Jan Storch

Our team's vision is to advance the field of organic and hybrid materials by synthesizing and applying polycyclic aromatic compounds, specifically [*n*]helicenes, and [*n*]phenacenes. We will prepare extended polyaromatics with D₂ and D₄ symmetry to increase g_{LUM} and investigate transition metal (Ln) complexes of [*n*]helicenes and chiral covalent organic frameworks to enhance circularly polarized light emission. We will produce and characterize new plasmonic hybrid optical materials to improve light-matter interaction and manipulation with circularly polarized light. Additionally, we will synthesize and test small hetero (N, P, O) systems for use in organic radical batteries and advance the field of energetics.

Team name: [Research Group of Bioorganic Chemistry and Biomaterials](#) | **Team leader:** Jindřich Karban

Our team's vision is advancing biomedical and biomaterial research through the synthesis and evaluation of glycomimetics, glycodendrimers, and dendrimersomes. These compounds have applications as advanced research tools in glycoscience and as drug candidates for the treatment of fibrotic and viral diseases, and cancer. We aim to develop inhibitors of carbohydrate-binding proteins with improved potency, selectivity, and pharmacological properties compared to unmodified endogenous carbohydrates. This includes the presentation of glycomimetics in multiple copies with tailored spatial distribution via attachment of glycomimetics to dendritic and supramolecular supports. The use of advanced modular synthesis will enable us to prepare tunable dendritic and supramolecular carriers for improved targeted internalization into cells and tissues. Additionally, we will synthesize a library of regioselectively modified polysaccharide segments to understand the structure-property relationships in polysaccharides. Detailed characterization of glycomimetics and their interactions with relevant biological targets will be achieved using advanced synthetic, physico-chemical, and computational methods.