INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS OF THE CAS, V. V. I.

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Institute of Chemical Process Fundamentals of the CAS, v. v. i.
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Contents

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GENERAL INFORMATION

The Institute of Chemical Process Fundamentals (ICPF) is one of six institutes constituting the Section of Chemical Sciences of the Czech Academy of Sciences. The Institute serves as a centre for fundamental research in chemical, biochemical, catalytic, and environmental engineering. Besides these activities, the Institute acts as a graduate school for Ph.D. studies in the field of chemical, biochemical, environmental engineering and processes, physical chemistry, organic chemistry, industrial chemistry, and biotechnology.

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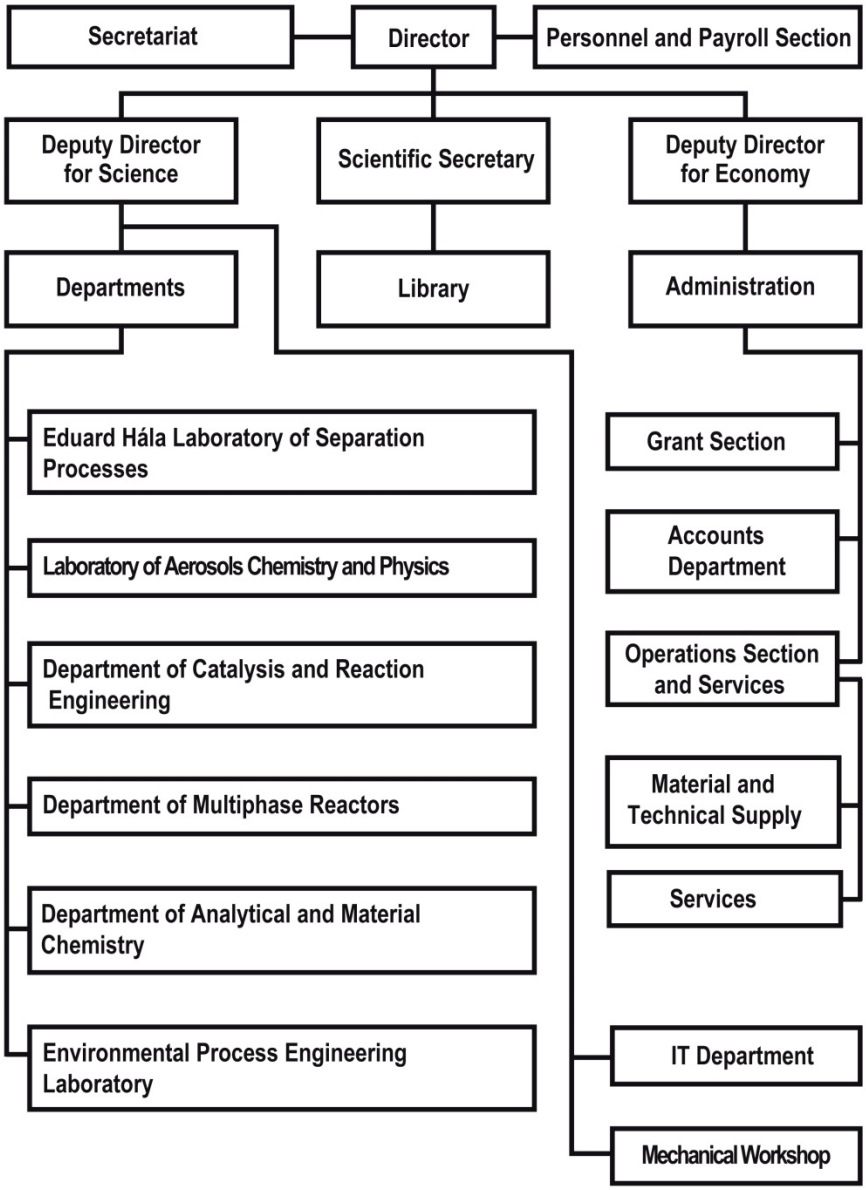
Organization Chart



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STAFF

(December 31, 2014)

Category	Number of Employees
Research	80
Research Support	67
Technical	10
Administrative	14
Services	10

BUDGET 2014

(20.75 CZK ≈ 1 US$, 27.53 CZK ≈ 1 €)

Resources	Million CZK
Institutional support based on Institutional Research Plan	75
Targeted support from Grant Agencies and R&D Programs in the Czech Republic	65
Foreign R&D Funds and European Programs	10
Contracts with industry	6
Other resources	14
Total Resources	**170**

Expenses	Million CZK
Personal expenses including mandatory insurance	100
Purchase of material	19
Purchase of services	6
Repairs and maintenance	9
Depreciation of fixed assets	15
Travel expenses	3
Energy, water, and fuels	4
Total other expenses	11
Total other expenses	**167**

Profit	Million CZK
Total	**3**

Eduard Hála Laboratory of Separation Processes

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PAVEL IZÁK

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LAB TECHNICIANS
MARTA KOPTOVÁ, **DALIBOR VLČEK**

Fields of research

- Thermophysical properties of pure ionic liquids and their liquid phase behaviour in mixtures with molecular solvents
- Experimental determination of vapour-liquid equilibria in mixtures containing components of low and high molecular mass
- Data processing using activity coefficient models and equations of state
- Prediction of phase behaviour by means of models based on group contribution methods
- Mass transport in polymeric membranes, mutual influence of permeating substances
- Membrane separation of CH_4 and CO_2 mixtures
- Separation of gases by ionic liquids membranes
- Condensation in porous membranes during vapor permeation
- Gas transport in asymmetric porous membranes
- Pervaporation - dehydration of alcohols, separation of azeotropic mixture, etc.
- Separation of volatile organic compound from air
- Pertraction – separation of enantiomers
- Evaluation of transport properties such as permeability, activation energy of permeation and selectivity of process
- Supercritical fluid extraction and pressurized liquid extraction of bioactive compounds from plants and their mathematical modelling; integration of extraction and fractionation

- Study on preparation of nanostructured metal oxides using supercritical and pressurized fluids
- Study on preparation of polymeric foams by pressurization with supercritical CO_2 followed by rapid depressurization
- Design and construction of extraction units based on Vibrating Plate Extractor (VPE)
- Extractive separation of biologically active substances from plants and microalgae
- Kinetic studies of hydrogenation reactions in a packed-bed microreactor
- Utilization of microreactors as an efficient tool for photosensitive reactions

Applied research

- Technology for the preparation of molecularly imprinted polymeric materials
- Separation of unwanted components from raw biogas
- Separation of volatile organic compound from air
- Separation of racemic mixtures
- CO_2 extracts of insecticidal substances from plants for botanical pesticides
- Recovery of precious and special metals from waste electrical and electronic equipment using Vibrating Plate Extractor (VPE)
- Microtechnology application for kinetic studies and process intensification

Research projects

Enrichment of raw biogas by methane

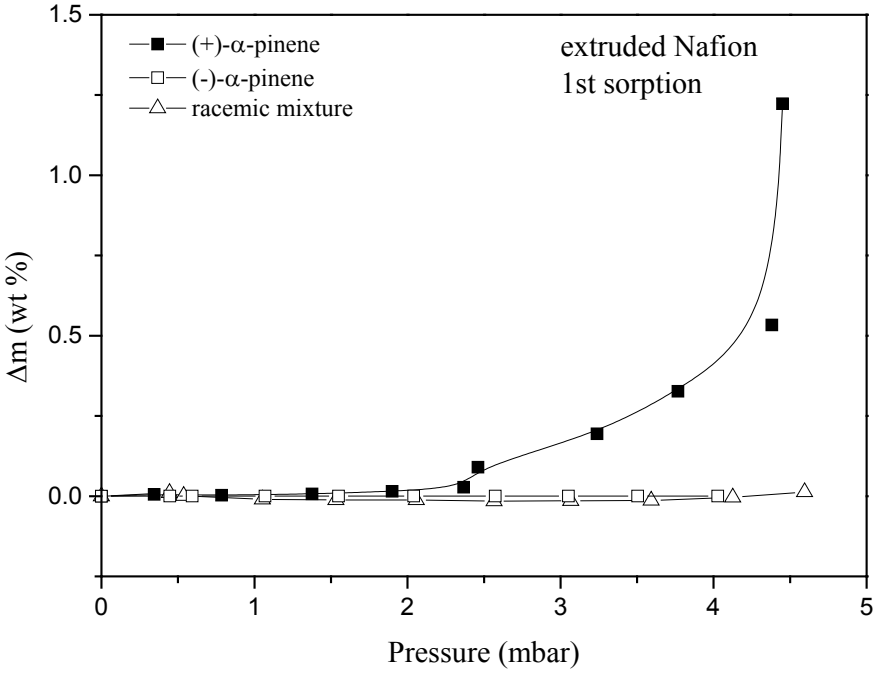
(P. Izák, izak@icpf.cas.cz; joint project with UCT, Prague; supported by MEYS, project No. LH14006)

The principal aim of this project is preparation, characterization and testing of advanced separation polymeric membranes with enhanced performance containing anchored ionic liquids in a suitable non-porous polymeric membrane using (i) Van der Waals forces in coated (composite) porous asymmetric polymeric membrane or (ii) a covalent bond or (iii) high ionic liquid content cross-linked polymer gels. Preparation of such novel separation membranes is targeted for an efficient methane separation from biogas. It will also be developed a model enabling prediction the transport and separation characteristics of these membranes intended for separation of gas mixtures. [Refs. 2, 21]

Membrane separation - the more effective separation of a pure enantiomer from a racemic mixture

(P. Izák, izak@icpf.cas.cz; joint project with UCT, Prague and IMC; supported by GACR, project No. P106/12/0569)

The aim of this work was to elucidate the sorption of α-pinene in the membranes of solution-cast and melt-extruded Nafion. The extruded membrane was Nafion® 115 in H^+ form (DuPont). The cast Nafion membrane was prepared by casting from a 20 wt.% solution of Nafion® (H^+ form) in lower aliphatic alcohols and water. (+)-α-pinene, (−)-α-pinene and racemic mixture sorption isotherms were determined by a gravimetric method using the sorption balance. It was found that the sorption of α-pinene in the Nafion membrane is a stereoselective process. The sorption of α-pinene in cast Nafion is much higher than in extruded Nafion. The sorption of (+)-α-pinene in the extruded Nafion membrane is quite low while the sorption of (−)-α-pinene approaches zero. The sorption of (−)-α-pinene in the cast Nafion membrane is high while the sorption of (+)-α-pinene is low. [Refs. 8, 12]

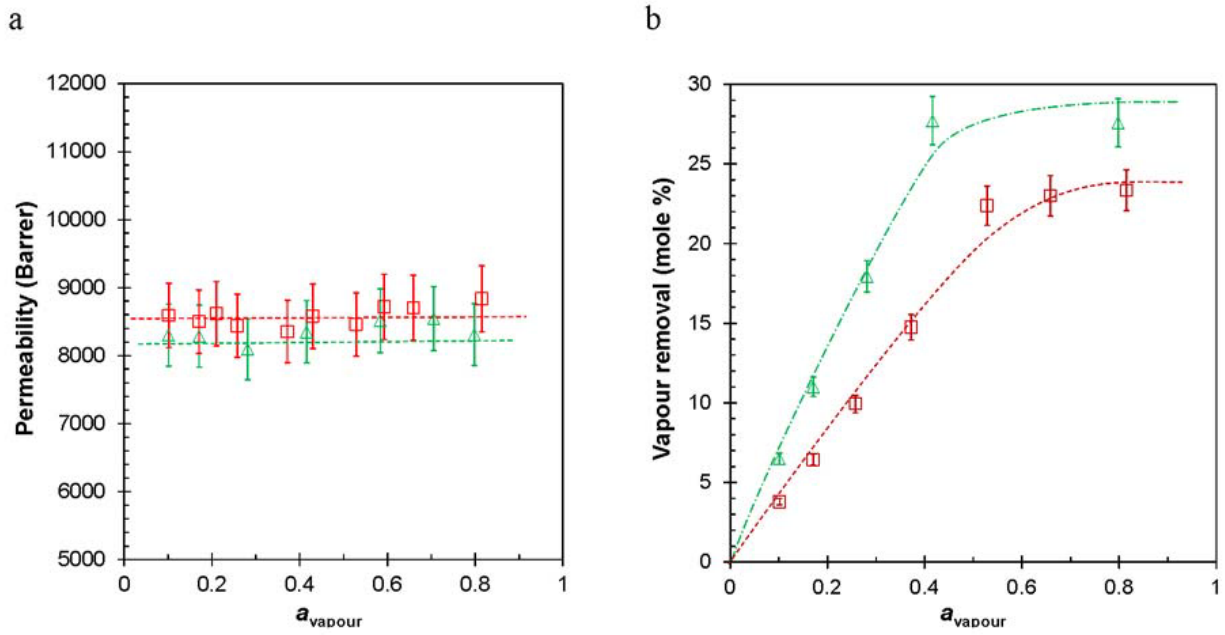


Sorption isotherms of (+)-α-pinene, (-)-α-pinene and their racemic mixture in extruded Nafion - the first sorption run

Supported ionic liquid membrane for separation of volatile organic compounds and pollutants from flue gases

(P. Izák, izak@icpf.cas.cz; supported by MEYS, project No. LD14094)

The aim of proposed project is the development of ionic-liquid containing membranes for the separation of volatile organic compounds and pollutants from flue gases. Also development of the model, which allows testing hypotheses about non-constancy of membrane characteristics along its surface and its possible dependency on various parameters, is part of the project. By comparison of experimental data with the model will also be validated. The validated model will be then used for the supported room temperature ionic liquid membrane optimization of its operating parameters and geometry. [Refs. 10, 13]

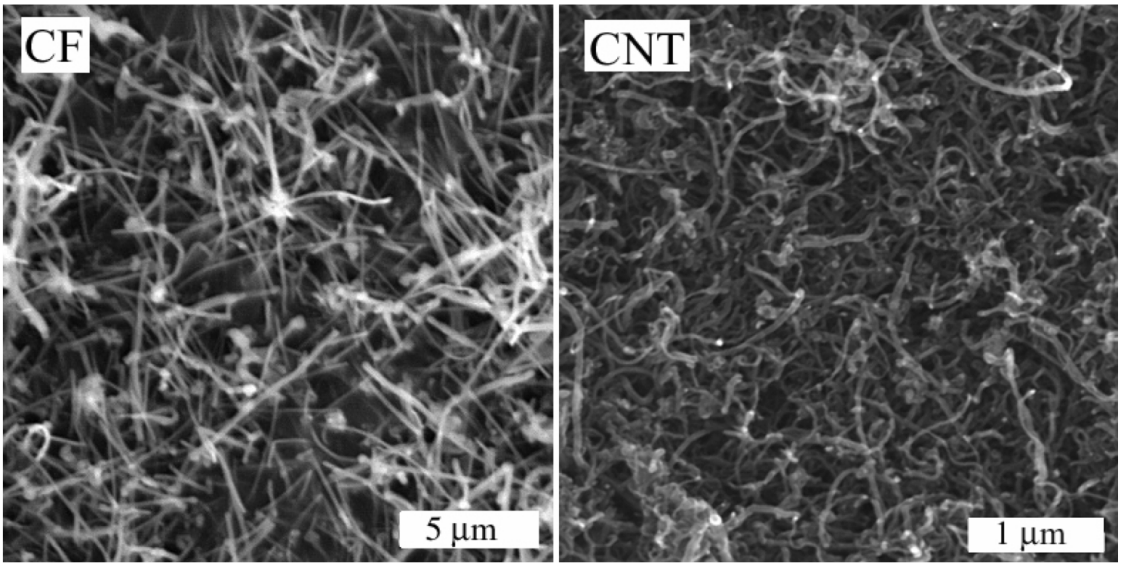


Comparison of permeabilities (a) and corresponding vapour removal (b) for hexane (Δ) and isooctane (□) at 35°C (lines are plotted to guide the eye)

Separation of polar and non-polar gasses by membrane processes

(P. Izák, izak@icpf.cas.cz; supported by GACR, project No. GA14-12695S)

The use of upgraded biogas is considered as one of the most efficient means of utilizing renewable and sustainable energy. Replacing of conventional methods by low-costs, membrane separations is therefore of a great interest. The aim of this project is to develop innovative highly selective membranes with improved performance for efficient biogas upgrading. Two parallel approaches of unique membrane preparation will be used: (i) the supported ionic liquid membranes and (ii) the water-swollen thin film composite membranes. A complementary and multidisciplinary approach to laboratory experiments for gas separation can be provided by modeling, which can pre-select the best ionic liquid and safe a lot of experimental work. The aspect connected with designing, preparation, characterization and evaluation of membranes for efficient biogas upgrading will be addressed to achieve the most successful membrane. The major issues are achieving high selectivity towards the target gas (methane) and testing this new separation method also for other polar gasses. [Refs. 7, 15, 19]



Scanning electron microscopy analyses of used fillers: carbon fibers (CFs) and carbon nanotubes (CNTs) [Ref. 15]

Permeation of condensable gases trough asymmetric membranes

(J. Řezníčková, reznickova@icpf.cas.cz; joint project with Institut für Strömungsmechanik und Wärmeübertragung Technische Universität Wien; supported by MEYS, MOBILITY, project No. 7AMB14AT011)

The aim of our collaboration is to carry out a series of experiments to obtain the pressure and temperature distributions within asymmetric ceramic membranes. The experimental data will improve our understanding of the permeation process especially under condition of condensation. It is difficult to set and maintain the correct experimental conditions. Furthermore, the direct measurement of the temperature and pressure distributions is not possible. Experimental difficulties are one of the reasons for the lack of sufficient experimental data. Therefore, a special apparatus was designed and constructed. The use of this apparatus will help at obtaining at least in an indirect way the desired pressure and temperature distributions. The data gleaned from our experiments will help at understanding the flow process. By condensation it may be possible to enhance the production in similar processes. [Ref. 17]

Preparation and characterization of mixed matrix membrane for gas separation

(P. Uchytil, uchytil@icpf.cas.cz; joint project with Department of Occupational Safety and Health, Chung Medical University, Taiwan, supported by CAS, PPP project, project No. MOST/14/02)

A nano-network TiO_2 intermediate layer was synthesized via a sol-gel method for fabricating a sandwich carbon molecular sieving (CMS) membrane with high separation performances for the H_2/CH_4 and H_2/CO_2 gas pairs. The effects of the TiO_2 nano-network preparation variables, including acid catalyst amounts and number of coats, on the structure of alumina support were evaluated. By adjusting the hydrolysis-condensation rate of the titania precursor using acid catalysts, control of the pore structure and roughness of TiO_2/Al_2O_3 composite supports could be achieved. Incorporation of a TiO_2 intermediate layer can also improve adhesion between the CMS layer and the support. Three techniques (field emission-scanning electron microscopy line scanning, Fourier transform infrared spectroscopy, and contact angle) were used to determine the individual contributions from mechanical

interlocking, from chemical bonding, and from the adsorption to adhesion mechanism. The sandwich CMS membrane follows the molecular sieving mechanism and exhibits the best values of 725.9, 8.3, and 87.9 for H_2/CH_4, H_2/CO_2, and CO_2/CH_4, respectively, with a H_2 permeability of 600.7 Barrer.

Applications of liquid-liquid extraction in recovery of precious and special metals

(A. Heyberger, heyberger@icpf.cas.cz; joint project with University of KwaZulu-Natal, Durban, Republic of South Africa)

On the basis of pilot plant experiments applied in recycling of luminophores from waste compact fluorescent light bulbs design of extraction unit with counter-current vibrating plate extractor (VPE) was proposed. Unit was constructed and operated at cooperating University. The pilot plant unit was designed universally for further adaptation to other similar hydro-metallurgical processes, e.g. recovery and purification of individual fractions of lanthanides from permanent magnets.

Pilot plant unit for recovery of luminophores in Durban

Research and development of new products for complex plant protection

(M. Sajfrtová, sajfrtova@icpf.cas.cz; joint project with Matoušek CZ a.s. and Crop Research Institute; supported by TACR, project No. TA01010578)

Supercritical extracts and hydrodistillates from tropical plants supplied from South Africa were produced to develop new protective preparations for eco-agriculture. The relationship extraction conditions - extract composition - pesticidal activity of extracts was examined for the supercritical fluid extraction and hydrodistillation and the optimal method and its conditions were determined for different effects against as the acute mortality, chronic mortality, antifeedance, and others. Several fractionation methods for dividing of the extract and increasing the concentration of different groups of active substances have been tested in laboratory scale [Ref. 14]. Mathematical description for scale up based on experiments conducted in laboratory and pilot plant apparatus was derived for the eucalyptus extraction.

Schema of development of new protective preparations for eco-agriculture

Unconventional preparation of nanostructured metal oxides by using pressurized and supercritical fluids

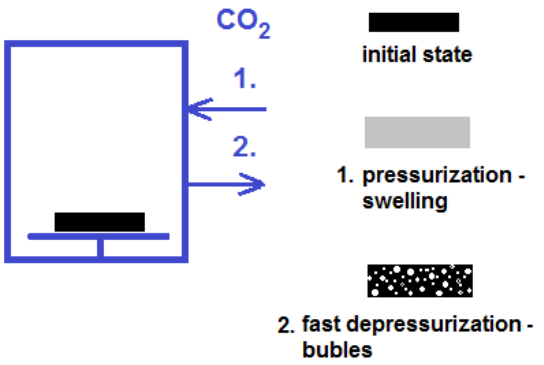
(M. Sajfrtová, sajfrtova@icpf.cas.cz; joint project with Nanotechnology Centre, VSB-TU Ostrava and X-ray group of Faculty of Mathematics and Physics, CU, Prague; supported by GACR, project No. GA14-23274S)

The project deals with investigation of preparation of various macroscopic forms (powders, thin films, monoliths) of nanostructured materials based on TiO_2, CeO_2, ZrO_2 and ZnO using sol-gel processes, thermal hydrolysis and extraction techniques developed for purpose of oxides purification and direct crystallization. Besides extraction by pressurized water and/or by super/subcritical methanol, also extraction by supercritical carbon dioxide with modifier/s is tested and optimized in a broad range of experimental conditions. The influence of individual types of extraction approaches and experimental conditions on microstructure is examined.

Morphology evolution of nano- and micro-cellular polymeric foams

(H. Sovová, sovova@icpf.cas.cz; joint project with Faculty of Chemical Engineering, UCT Prague and New Technology – Research Centre, University of West Bohemia, supported by GACR, project No. GA14-18938S)

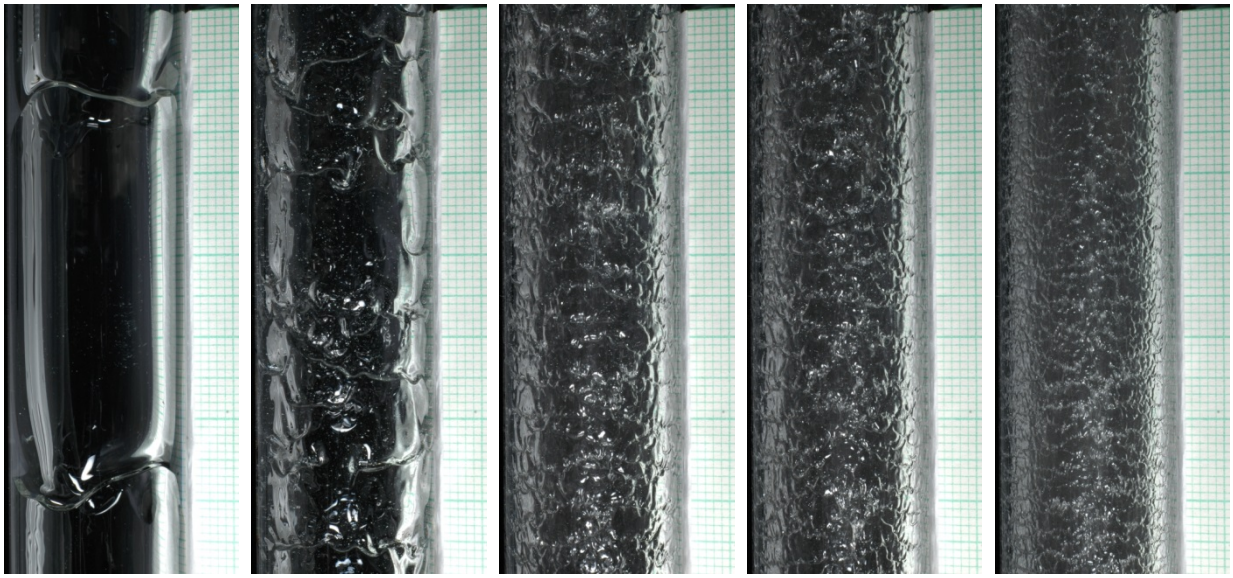
The project is aimed at first-principles understanding of early stages of polymer foam evolution including nucleation or phase separation by spinodal decomposition and coalescence of cells. Experimental methods include, among others, the foaming of polystyrene with supercritical CO_2. Based on the improved understanding of nucleation and coalescence, the methods of nano-/micro-cellular foam preparation will be assessed and optimized.



Pressure drop during the annular gas-liquid flow

(J. Křišťál, kristal@icpf.cas.cz; research contract with Procter&Gamble)

This project followed our cooperation with Procter&Gamble established during previous EU projects (IMPULSE, F^3 Factory) and research contracts. The objective of the project was a hydrodynamic study of annular gas-liquid flow. Range of operation of the existing experimental unit was extended to accommodate the reactors with different inner diameter. Wide range of experiments was carried out in order to correlate a pressure drop and a flow regime with gas and liquid velocities.



v_G = 6.4 m/s v_G = 19.1 m/s v_G = 50.6 m/s v_G = 63.3 m/s v_G = 96.1 m/s

Flow regime visualization of annular gas-liquid flow

Consulting and support on microProcessing capabilities

(J. Křišťál, kristal@icpf.cas.cz; research contract with Procter&Gamble)

Procter&Gamble was interested in our know-how accumulated about the microreactor technology application for process intensification. The work consisted in an efficient information exchange and support in various fields of microprocessing.

Application of microreactors for gas phase catalytic reactions

(P. Stavárek, stavarek@icpf.cas.cz; research contract with Momentive Specialty Chemicals a.s.)

The feasibility of application of microreactors was assessed and evaluated for the gas phase catalytic oxidation reaction. Based on this feasibility study, the preliminary design of an experimental laboratory apparatus was prepared. The work followed with a detailed design of a laboratory microreactor and the whole apparatus (under construction now) to create a basis for future laboratory testing, which will enable even widening of our current cooperation.

Development of advanced separation methods for liquid-liquid systems

(J. Křišťál, kristal@icpf.cas.cz; research contract with: Modelarna LIAZ s. r. o.)

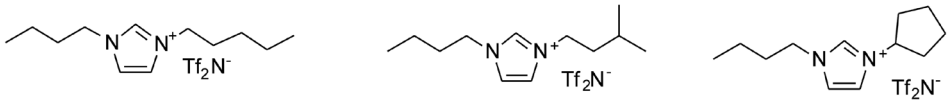
The objective of this project was the development of advanced separation methods for mixtures of miscible liquids and its experimental validation. For this purpose a laboratory apparatus was constructed and a wide range of tests were performed. The collected results provided a basis for a common patent application. [Ref. 3]

Branched and cyclic alkyl groups in imidazolium-based ionic liquids: Molecular organization and physico-chemical properties

(M. Bendová, bendova@icpf.cas.cz; joint project with Equipe Thermodynamique des Intéractions Moléculaires, Institut de Chimie de Clermont-Ferrand, Université Blaise Pascal, France)

Novel $[C_4C_5Im][Tf_2N]$ ionic liquids with a variation in structure of a C5 alkyl group were synthesized for the first time and characterized as to their thermophysical and transport properties. Branching of the alkyl chain has no influence on the ionic liquid density. Isopentyl

and cyclopentyl groups increase the ionic liquid viscosity. Surprisingly the cyclopentyl substituted ionic liquid shows the highest conductivity in spite of its high viscosity. This however is in agreement with a higher degree of its ion dissociation found from the experimental self-diffusion coefficients. [Refs. 1, 9]

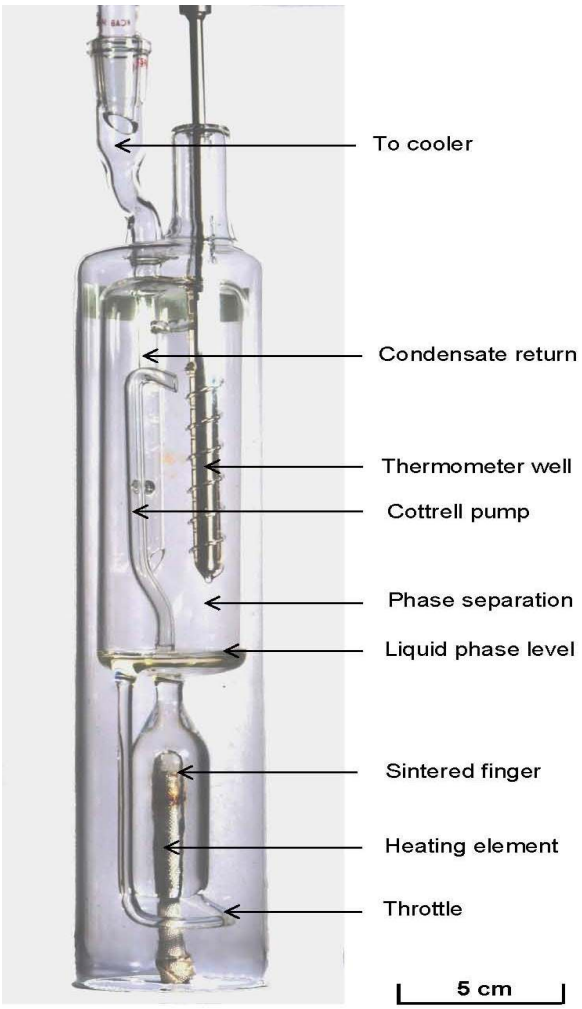


Structures of the 1-alkyl-3-butylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids

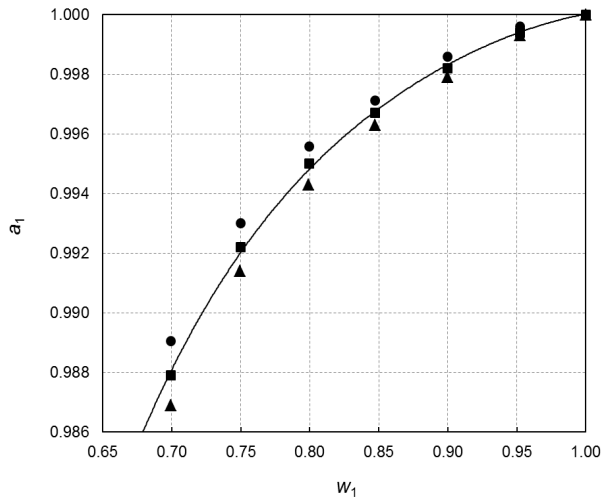
Vapour-liquid equilibrium in systems containing polymers - measurement and data processing

(I. Wichterle, wichterle@icpf.cas.cz; within the project "Group of phase equilibria" supported by ICPF)

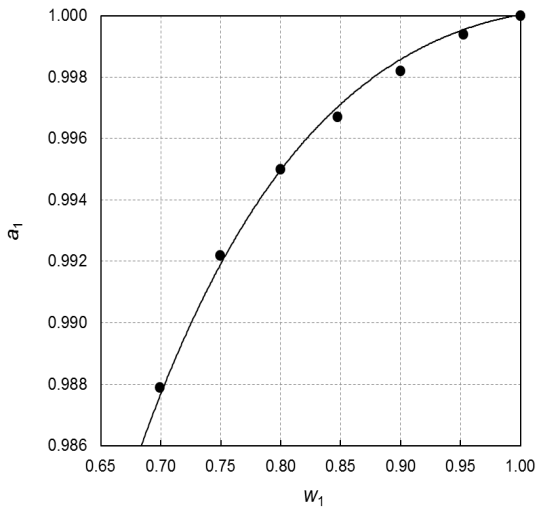
Vapour-liquid equilibria have been determined in systems composed of poly-(acrylic acid) with water, and poly(methyl methacrylate) with 2-butanone by ebullio-metric (total pressure measurement) method. Ebulliometer has been redesigned (see the Figure) and experimental procedure has been upgraded. Experiments have been carried out isothermally, the measured data were correlated by the UNIQUAC-FV model, and compared with available literature data. It should be stressed that this type of measurements, *i.e.* ebulliometry in the high-concentration region of solvent, is unique and is presently carried out only at the ICPF. The polystyrene + toluene system has been measured, too (paper published in 2015). Results were published in journal [Ref. 11] and at two international confe-rences.



Microebulliometer – new design



Activity a1 of 2-butanone in PMMA as a function of 2-butanone mass fraction w1. Experimental data at (•) 333.15 K, (■) 343.15 K and (▲) 353.15 K. Solid line represents predicted activities at 343.15 K using the UNIQUAC-FV parameters estimated using all data within temperature range 333.15–353.15 K



Activity a1 of 2-butanone in PMMA as a function of 2-butanone mass fraction w1. Experimental data at (•) 343.15 K. Solid line represents predicted activities using UNIFAC-vdw-FV model

International co-operations

CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials

Institut für Strömungsmechanik und Wärmeübertragung Technische Universität Wien: Flow of saturated vapors through porous membranes

Institute of Chemical Engineering, Sofia, BAS: High-pressure phase equilibria

Institute of Macromolecules, St. Petersburg, RAS, Russia: Membrane separation

Institute on Membrane Technology, CNR, Italy: Novel composite membranes containing ionic liquid and selected polymers for specific gas/gas, gas/vapor and vapor/vapor separations

KIT Karlsruhe, Germany: Design of pilot plant size microreactor for sulfur dioxide catalytic heterogeneous oxidation

Momentive Specialty Chemicals, Czech Republic: Application of microreactors for gas phase catalytic reactions

National Chung Hsing University, Taiwan: Preparation of Dense Homogeneous Polymeric Membranes and Study on Their Gas Permeation Properties

New University of Lisbon, Portugal: Membrane separation processes

Otto von Guericke University of Magdeburg, Germany, Max-Planck-Institut für Dynamikkomplexer technischer Systeme. Magdeburg: Mass transport through porous membranes

Procter&Gamble, Belgium: Research and developments of microapparatus characteristics

Procter&Gamble, Belgium: Hydrodynamics of micro reactor for sulfonation

Procter&Gamble, Belgium: Hydrodynamics of annular gas-liquid flow

Swiss Federal Institute, Switzerland: Chiral ionic liquids and membrane separation

Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapors through porous membranes

Technical University of Lisbon, Portugal: Supercritical extraction of biological compounds from aromatic plants
University of Colorado, Boulder, CO, USA: Mass transport during vapor permeation and pervaporation, ionic liquids
University of Burgos, Spain: Enzymatic reactions of oil in supercritical CO_2 medium
University of KwaZulu-Natal, Republic of South Africa: Liquid-liquid extraction processes with fluorinated hydrocarbons, recovery of luminophores

Visitors

Prof. A. Seidel-Morgenstern, University of Magdeburg, Max-Planck Institute, Germany
Dr. Thomas Loimer, Technische Universität Wien
Prof. H-H. Tseng, Chung Medical University, Taichung, Taiwan
Dr. S. Kononovou, Institute of Macromolecular Compounds, Russian Academy of Sciences, Saint-Petersburg, Russia

Teaching

J. Hanika: UCT, Faculty of Chemical Technology, postgradual course “Multiphase Reactors”
J. Hanika: UCT, Faculty of Chemical Technology, course “Pharmaceutical Engineering”
H. Sovová: TU Darmstadt, Life Long Intensive Program “Process Intensification by High Pressure Technologies – Actual Strategies for Energy and Resources Conservation”
M. Bendová: UCT, Faculty of Chemical Engineering, postgraduate course "Physical Chemistry for Technological Practice"
Z. Sedláková: UJEP, Faculty of Science, courses "Membrane Separations", "Basic of Chemistry", "Laboratory of Analytical Chemistry"

Publications

Original papers

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Fields of research

- Atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- Heat and mass transfer in aerosol systems
- Interaction of aerosols with electromagnetic radiation
- Emissions sampling
- Engineered nanoparticles and health
- Aerosol technology
- Density functional study of interfacial phase transitions and nanodrops
- Dynamic properties of simple and complex fluids on a molecular scale
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Development of equations of state based on molecular theory
- Molecular simulations of solid–liquid interfaces
- Mesoscale simulations of polymeric and energetic systems
- Density functional study of interfacial phase transitions and critical phenomena at non-planar surfaces
- Dynamic non-equilibrium properties of complex fluids and their mixtures

Research projects

Molecular-level simulations aqueous electrolytes

(I. Nezbeda, ivonez@icpf.cas.cz; joint project with the University of Ontario, Institute of Technology, Oshawa, ON, Canada and UJEP; supported by UJEP)

This series of papers deals with common non-polarizable models of electrolytes with the goals to (i) assess their appropriateness, (ii) find ranges of their applicability, and (iii) examine the possibility of their improvement by a reparametrization. Consistency tests of available literature data for the chemical potential were also performed. All simulations used the recently developed MPM-MC method demonstrating thereby its efficiency. [Ref. 3]

Tailored self-assembly of polyelectrolyte copolymers with surfactants in aqueous solutions

(Z. Posel, M. Lísal, posel@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-02938S)

Multidisciplinary study of the tailored self-assembly of branched polyelectrolyte copolymers with surfactants in aqueous solutions aimed at deeper understanding of the relationship between the chain architecture and the structure, stability, thermodynamic behavior and properties of nanostructures formed under different conditions (pH, ionic strength, temperature) was carried out. A combination of dissipative particle dynamics and newly developed hybrid Monte Carlo method with experiments was used. [Refs. 20-22]

A controlling of diffusion processes in pores with varying permeability

(A. Malijevský, M. Lísal, malijevsky@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-09914S)

Interfacial phase transitions at non-planar surfaces have been studied in the framework of a density functional theory and effective Hamiltonian theory. New hidden connections (covariances) between adsorption phenomena at different substrate geometries have been found and explained. While most of the results obtained by the two theories give mutually consistent conclusions, the molecular-based density functional theory whose implementation was newly extended for the geometries possessing nontrivial symmetries, provides a more microscopic insight into the understanding of the interfacial phenomena and revealed some new and surprising predictions. These results are not only interesting by their own rights but also serve as a pre-requisite for a further study of dynamical properties of fluids (such as diffusive processes) at modified surfaces and between patterned walls. [Refs. 14-16]

Mesoscopic modeling of protein - surface interactions

(A. Malijevský, Z. Posel, and M. Lísal, malijevsky@icpf.cas.cz, posel@icpf.cas.cz, and lisal@icpf.cas.cz; supported by Grant Programme of the MEYS, project No. LH12020)

Mesoscopic modeling using dissipative particle dynamics was employed to systematically study the effect of shape, size and hydrophobicity / hydrophilicity of proteins on their adsorption kinetics. Mesoscale models of proteins and surfaces were obtained from atomistic simulations of individual proteins in water and individual proteins close to walls using mapping from the atomistic to mesoscopic level. [Refs. 5, 12]

Mesoscale Modeling of Dynamic Response of Reactive Materials

(M. Lísal, lisal@icpf.cas.cz; supported by Cooperative Agreement W911NF-10-2-0039)

The Dissipative Particle Dynamics method was extended to simulate chemical reactivity (DPD-RX) of multi-step decomposition reactions, and was applied to a thermally-initiated RDX decomposition reaction model. For the DPD-RX methodology

extended to multi-step reactions, a coarse-grain particle equation-of-state (CG-EOS) was further developed based on the internal partition function, which accounts for the standard-state contributions in a thermodynamically-consistent manner. Finally, the gas expansion that follows RDX decomposition was captured via composition-dependent particle interactions based upon a one-fluid approximation. [Refs. 2, 7, 8]

Human EXposure to Aerosol COntaminants in Modern Microenvironments

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, Marie Curie Actions - Initial Training Networks, project No. 315760, FP7-PEOPLE-2012-ITN, HEXACOMM, project partner)

The main research goal of HEXACOMM is to apply scientifically-based modelling and experimental methods to relate concentrations of particulate matter in the indoor domestic environment to its sources and human exposure implications. The second research objective is to determine the human exposure arising from such exposure at both individual and collective (population) scales at modern microenvironments.

Contributions from outdoor air will be taken into account. Central idea of HEXACOMM is that a combination of tools and methods will enable us to relate indoor air quality to aerosol contaminants in urban homes, offices, vehicles with human exposure in a quantitative manner. To achieve our goal and objectives we propose to undertake, in parallel, a carefully designed validation programme at the European scale combining specifically targeted indoor air quality measurements, source apportionment studies, micro-environmental modelling, dosimetry modelling and exposure studies. Ultimately, our vision is that such enhanced understanding of the underpinning science will lead to improved indoor air quality in European domestic environments, while facilitating development of strategies to mitigate the impacts of aerosols on human exposure. [Ref. 4]

Aerosols, Clouds, and Trace gases Research Infra Structure Network

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, project No. INFRA-2010-1.1.16 ACTRIS, as “initial associated partner”)

ACTRIS (Aerosols, Clouds, and Trace gases Research Infra Structure Network) is an European Project aiming at integrating European ground-based stations equipped with advanced atmospheric probing instrumentation for aerosols, clouds, and short-lived gas-phase species. ACTRIS will have the essential role to support building of new knowledge as well as policy issues on climate change, air quality, and long-range transport of pollutants.

ACTRIS is building the next generation of the ground-based component of the EU observing system by integrating three existing research infrastructures: EUSAAR, EARLINET, CLOUDNET, and a new trace gas network component into a single coordinated framework. ACTRIS is funded within the EC FP7 under "Research Infrastructures for Atmospheric Research". [Refs. 1, 17]

Centre for studies on toxicity of nanoparticles

(P. Moravec, moravec@icpf.cas.cz; supported by GACR, project No. P503/12/G147)

The rapid expansion of nanomaterials production and their use in many products create a need for understanding the mechanisms of nanomaterial interactions with living systems. This need is above all given by unique properties of nanoparticles related to their dimensions and by their ability to penetrate into various tissues and cells in organism. Nanoparticles are also formed unintentionally as a result of the anthropogenic activities (industry, local heating). The proposed interdisciplinary centre of basic research will integrate laboratories capable to perform complex studies on mechanism of the toxicity of important and widely used engineered nanoparticles, as well as anthropogenic nanoparticles in the environment with a special attention paid to heavily polluted areas of the Czech Republic. The studies will be

performed on thoroughly characterized nanoparticles to obtain valid and comparable results on biological action and toxicity of nanoparticles.

Advanced study of physical and chemical properties of atmospheric aerosols in high time resolution

(V. Ždímal, zdimal@icpf.cas.cz; supported by GACR, project No. 209/11/1342)

Advanced physical and chemical properties of Central European atmospheric aerosol at rural background and urban background sites will be studied in high time and size resolution. Parallel measurement of aerosol volatility will be carried out using a C-ToF-AMS equipped with a thermodenuder inlet, aerosol hygroscopicity using a Hygroscopic Tandem Differential Mobility Analyser (HTDMA), and particle number size distribution using a Scanning Mobility Particle Sizer (SMPS). The information about aerosol particle density will be extracted from the SMPS and AMS. Hygroscopicity closure will be obtained from the combined HTDMA and AMS chemical composition data allowing to study the influence of organic aerosol on particles' hygroscopicity. The content of primary and secondary organic aerosol and the extent of aerosol ageing will be determined using AMS data at each site. In addition, at least a year-long time evolution of number size distributions obtained using the SMPS and OC/EC concentrations from the OC/EC analyzer will be delivered to the EBAS database, to be available for global atmospheric modeling groups. [Refs. 26-29]

Thermophysical properties of water in unexplored, technologically significant regions

(V. Ždímal, zdimal@icpf.cas.cz; joint project with Institute of Thermomechanics of the CAS, CTU, and University of West Bohemia, Plzeň; supported by GA ASCR, project No. IAA4200760905)

This project focuses primarily on liquid water and solutions of selected salts below the freezing point (supercooled water), and water in nano-droplets. Existing hypotheses include the possibility of phase separation of supercooled water into two liquid phases below the second critical point. Density of supercooled water is only known at 0.1 MPa. Suggested measurements up to 100 MPa will provide first data. A new method and apparatus will be developed. The surface tension of supercooled water and a salt solution will be measured. The surface tension of nano-droplets will be estimated from nucleation experiments. A range of theoretical approaches including phenomenological methods, simplified microscopic models, and molecular simulations, will be used with experimental data to obtain fundamental findings and engineering models. [Ref. 23]

Development and application of new experimental methods to measure heterogeneous particles in superheated steam

(V. Ždímal, zdimal@icpf.cas.cz; joint project with CTU and Institute of Thermomechanics of the CAS; supported by GACR, project No. 101/09/1633)

The aim of the project is to determine some properties of heterogeneous nuclei present in the superheated steam of steam turbines. In this project, the sampling device, coupled to advanced aerosol instrumentation (condensation particle counter, scanning mobility particle sizer), will be used to measure heterogeneous particles at selected power stations. To enable measurements of particles down to about 1 nm, a fast expansion chamber will be developed, enabling resolution of particle size by variable supersaturation. Collected data will serve as a basis for understanding the transport and the state of agglomeration of chemicals present in the steam circuit, for quantifying their effect on condensation, and, consequently, on the efficiency and reliability of steam turbines. [Ref. 6]

Black and elemental carbon at two European urban sites – site specific similarities and differences in method intercomparability

(J. Schwarz, schwarz@icpf.cas.cz; supported by MEYS, program MOBILITY, project No. 7AMB12AT021)

The method intercomparison studies will be conducted both under summer and winter conditions at both sites lasting 2 weeks each. By pooling the instruments and expertise of the two partners, BC will be measured on-line with the MAAP and the aethalometer techniques and from filter samples with the integrating sphere technique; EC will be investigated both from bulk samples with a Sunset Analyzer set both in reflection and transmission modes with three thermal protocols (NIOSH, DRI, EUSAAR2) and quasi on-line with two Sunset Field Analyzers set to two different temperature protocols. BrC will be analyzed with the modified integrating sphere technique. Background information on the aerosol will be obtained in parallel. [Ref. 28]

Methodology of evaluation of air quality effect on library and archival collections

(J. Smolík, smolik@icpf.cas.cz; supported by the Ministry of Culture of the CR, project No. DF11P01OVV020)

The aims of the project are: a) development of evaluation methods for indoor air quality in libraries and archives, targeted at reduction of damages on library and archival collections caused by adverse effects of environment and b) gaining detailed knowledge of direct dependences between damage of library and archival collections and surrounding environment, leading to precautions reducing the adverse effects of deteriorated environment. [Ref. 13]

International co-operations

Imperial College London, London, UK: Confined fluids
Penn State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behavior of model proteins on surface
University of Loughborough, Loughborough, UK: Dynamic density functional theory
University of Ontario Institute of Technology, Oshawa, ON, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids
U.S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale simulations of energetic and reactive materials
Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
Laboratory of Atmospheric Chemistry, Paul Scherrer Institute, Switzerland
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behavior
Technical University of Crete, Chania, Greece: Aerosols in the indoor environment
University of Helsinki, Division of Atmospheric Sciences, Helsinki, Finland
University of Vienna, Faculty of Physics, Dept. of Aerosol physics and Environmental Physics, Vienna, Austria: Black and elemental carbon analysis, aerosol optical properties

Visits abroad

D. Brus: Finnish Meteorological Institute, Helsinki, Finland (12 months)
M. Lísal: The University of Alabama, Tuscaloosa, AL, USA (1 month)
A. Malijevský: Imperial College London, London, UK (3 months)

Visitors

Coray M. Colina, Department of Materials Science, Penn State University, State College, USA

Teaching

V. Ždímal: Faculty of Mathematics and Physics, Charles University in Prague, undergraduate course: “Aerosol Engineering”

V. Ždímal: UCT, Faculty of Chemical Engineering, graduate course “Aerosol Engineering”

J. Jirsák: UJEP, Faculty of Science, courses "Introduction to Chemistry", "Physical Chemistry", "Physical Chemistry Seminar" and "Free Software in Natural Sciences"

M. Lísal: UJEP, Faculty of Science, courses “Parallel Programming”, “Numerical Mathematics”, “Molecular Simulations” and “Mesoscale Simulations”

A. Malijevský: UCT, Faculty of Chemical Engineering, courses “Physical Chemistry I”, “Physical Chemistry of the Micro-World", "Introduction to a Modern Theory of Phase Transitions", "Mathematics for Physical Chemistry" and "Statistical Thermodynamics", Molecular Simulations and Modelling

Publications

Original papers

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Chapters in books

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Fields of research

- Advanced catalytic oxidation processes
- Catalytic combustion of volatile organic compounds in waste gases
- Catalytic decomposition of N_2O
- Design of new theoretical models for structure-activity relationships
- Morphology and application properties of catalysts based on functional polymers
- Preparation of hierarchic nanomaterials
- Temperature programmed techniques in characterization of catalysts
- Texture and transport processes in porous solids
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Preparation and characterization of the electrospun nanofibrous membranes and catalytic supports
- Unconventional preparation of metal oxide nanostructures by pressurized fluid extraction and supercritical drying

Applied research

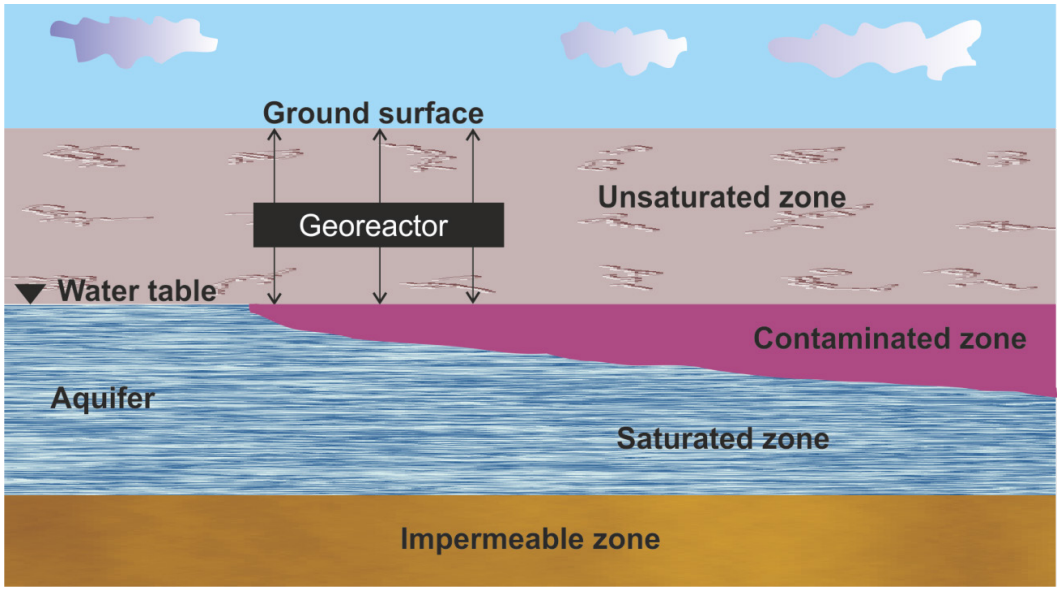
- Catalytic combustion of volatile organic compounds
- Oxidation processes for environment
- Textural characteristics of structural materials
- Green chemistry for biomass utilization to the high added-value products

Research projects

Hydrogen oriented underground coal gasification (UCG) for Europe - environmental and safety aspects (HUGE2)

(O. Šolcová, solcova@icpf.cas.cz; joint project with GIG, Politechnika Slaska, Kompania Węglowa S.A. and Lubelski Węgiel Bogdanka S.A., Poland, Institut National de l`environnement industriel et de risques, France and UCG Engineering Ltd, UK; supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2011-00002)

This project is focused on safety and environmental aspects of underground coal gasification. Underground trial has been performed in mine testing two borehole system and reactive barriers usage. The most serious environmental concerns related to UCG have been investigated that is contamination of underground aquifers and potential leakage of poisonous and explosive gates into the surrounding strata. The work is focused on finding practical solutions of possible leakages prevention by use of reactive barriers. Complex system of environmental telemetric monitoring was built and tested. Also technical and ecological risk assessment was performed.



Conceptual model of the contaminants migration from georeactor zone

HUGE2 project has played a complex role in the development of the UCG technologies, an important element of Clean Coal Technology proposals for Europe. It has enabled the enhancement of the consolidation between the European laboratories involved in the development of the UCG technology as well as comprised the continuation of collaboration established within the HUGE (2007-2010) project between the European experts and the European coal companies. Necessary attention has been paid to the implementation of the UCG technologies in industry through the involvement of companies, in particular from outside of Europe. The project has helped to overcome the legal and formal restrictions through enhancing the knowledge of the environmental constrains and hazards as well as providing the tools to help overcome these constrains. It has delivered the resources and opportunities for the development of the Clean Coal Technology Centre in the Central Mining Institute. It has enabled launching PhD courses within the Polish project – Development of human resources for Clean Coal Technologies' research. The HUGE2 project has become the vehicle for other European projects dedicated to Underground Coal Gasification such as: Technology Options for Coupled Underground Coal Gasification and CO_2 Capture and

Storage (TOPS), Enhanced Coal Exploitation through UCG Implementation in European Lignite Mines (Coal2Gas) and Methane Production through Underground Coal Gasification from Deep European Coal Seams (MEGA). [Ref. 15]

Removal of heavy metals and radionuclides from water using ceramic membranes

(O. Šolcová, solcova@icpf.cas.cz; joint project with Institute for Single Crystals of NAS of Ukraine and University of Maribor, Slovenia; supported by NATO, project No. SFP 984398)

The problem of environmental pollution with radionuclides is especially acute in Ukraine after the Chernobyl catastrophe in 1986 which caused serious radioactive contamination of the surface aquatic environment. Even currently uranium concentration in liquid low-level radioactive wastes from the object "Shelter" in Chernobyl Exclusion Zone exceeds 30-40 mg/l. These wastes require treatment to meet discharge regulations to the inland waterways and to minimize the volume of radioactive material to be stored. Additionally, Ukraine ranks sixth place in the world and first in Europe regarding the reserves of uranium ores. Large volumes of drainage and process water contaminated with uranium and other radionuclides are formed during mining and enriching of uranium ores. Unfortunately, this polluted water as a rule enters the environment without adequate treatment.

Therefore, the main objective of the project is to develop a family of advanced nano- and ultrafiltration ceramic composite membranes containing functionalized mesoporous silica layers which will be capable of selective binding of heavy metals (Hg, Cd, Cr) and uranium from surface and waste waters and thus preventing or minimizing the environmental exposure to hazardous substances. [Ref. 19]

Structured catalysts with active oxide layer for removal of gaseous pollutants

(K. Jirátová, jiratova@icpf.cas.cz; joint project with TU of Ostrava, and UCT, Prague; supported by GACR, project No. 14-13750S)

Mechanochemical method was proposed and applied for preparation of Al-Ce mixed oxide supports of catalysts for the total oxidation of volatile organic compounds. The calcination products do not contain harmful sodium and show high surface area, large pore volume, and big average diameter of mesopores (around 8 nm). Analogous mechanochemical method was used for preparation of precursors giving the Co-Mn-Al mixed oxide catalysts after heating. The catalysts were modified with Cs promoter and showed high activity and selectivity in ammonia oxidation to N_2O at low temperatures of about 250 °C.

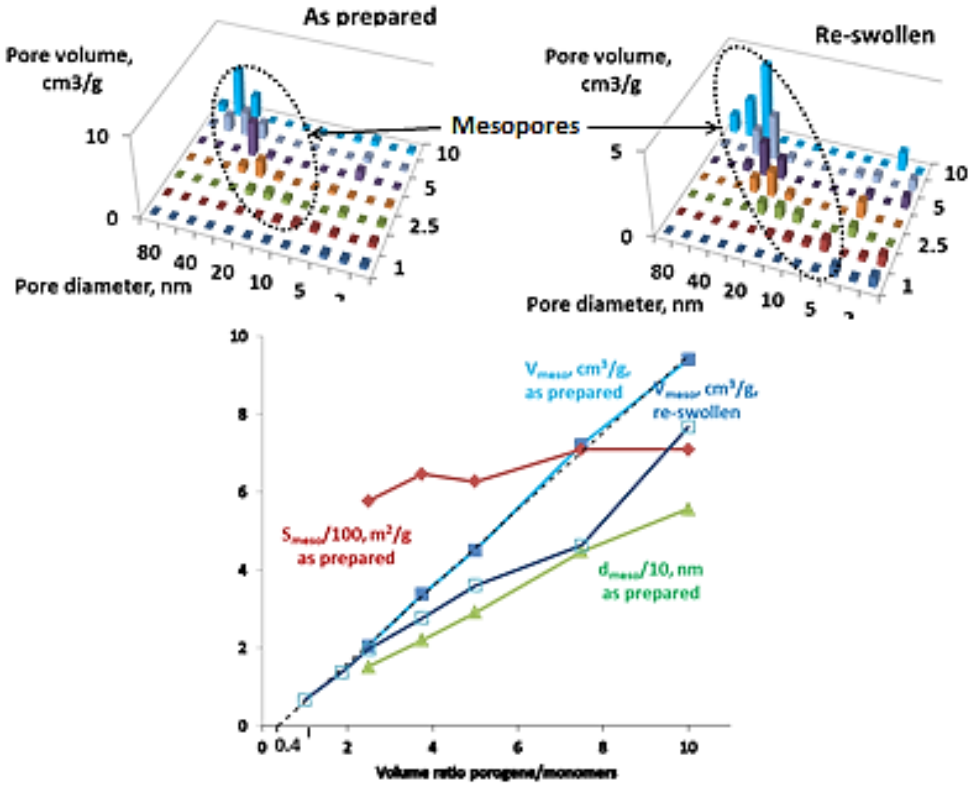
The Co-Mn-Al mixed oxide catalysts on preformed supports (alumina spheres and cordierite monoliths wash coated with alumina) were prepared and tested in the total oxidation of ethanol and decomposition of N_2O. The catalysts prepared by deposition of dried LDH precursor over alumina spheres showed the highest activity. The activity of monolithic catalysts was comparable to that of the impregnated pellets. The Co-Mn-Al mixed oxides were deposited on the supports by hydrothermal crystallization of LDH precursors and subsequent heating. The aluminum sieve and monolith with (Co+Mn) active metals exhibited comparable activity in ethanol oxidation as reference Envicat catalyst.

Morphology and application properties of mesoporous poly(divinylbenzenes)

(K. Jeřábek, kjer@icpf.cas.cz; joint project with Zhejiang University, Hangzhou, China; supported by MEYS, project No. LH12194)

Chinese colleagues discovered a novel polymerization method producing porous polymers with very high surface area and unique mesoporous morphology, completely different from conventionally prepared materials of similar chemical nature. In their preparation is used exceptionally high dilution of monomers with porogenic solvents. With help of inverse steric exclusion chromatography method developed in Prague providing

information on the polymer morphology in its native, swollen state undeformed are investigated relations between preparation conditions of mesoporous functional polymers and their morphology. It was found that the pore volume in the polymer examined just after preparation corresponded to the volume of the porogen used [Ref. 18]. Drying of the polymers of course induces extensive collapse of the porous structure. Water, as additive to the porogenic solvent, influences ability of the polymer morphology to re-swell to its original state. There was found that the mesoporous morphology is formed by microsyneresis rather than the macrosyneresis mechanism that is common in the synthesis of conventional porous polymer materials. There were defined conditions needed for the microsyneretic pore formation in highly crosslinked polymer materials allowing production of a new class of functional polymers. [Refs. 5, 6, 14, 18]



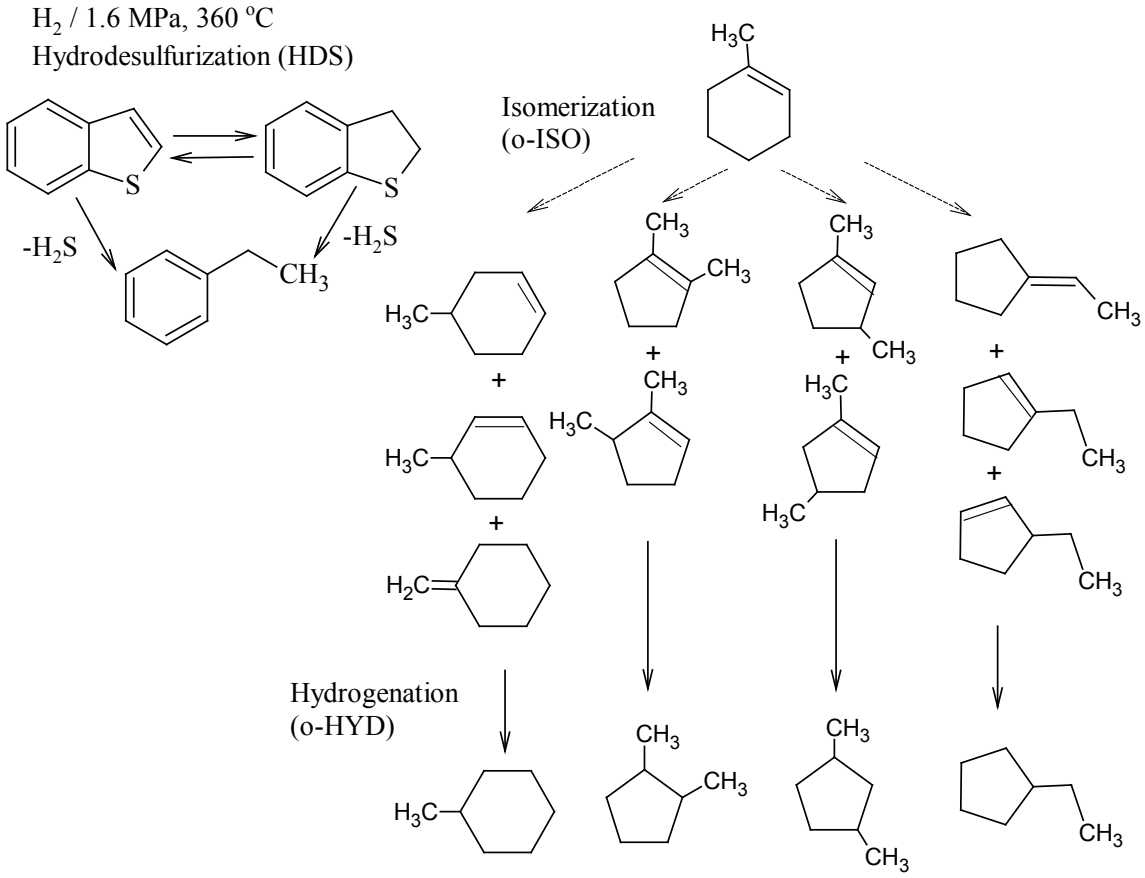
Effect of monomer dilution (tech. DVB, 80 %) with toluene on the swollen-state morphology assessed by ISEC

Unconventional composition and preparation of sulfide hydrotreating catalysts

(L. Kaluža, kaluza@icpf.cas.cz; supported by GACR, project No. 106/11/0902)

Sulfide $CoMo/Al_2O_3$ catalysts were compared with unconventional $PdMo/Al_2O_3$ in hydrodesulfurization (HDS) reaction of model compounds emphasizing on the catalysts nitrogen tolerance. Furthermore, the studies were focused on elucidation of the effect of catalyst precursor and its pretreatment on the amount of ß-Pd hydride phase and HDS activity over bimetallic Pd-Pt/silica-alumina. Over selected catalysts, moreover, the rearrangement of 1-methylcyclohex-1-ene during the HDS of model fluid catalytic cracking (FCC) gasoline was described. An isolation and identification of branched cyclic C7 olefins were addressed. Dimethyl-cyclopentenes and ethylcyclopentenes were determined during the simultaneous HDS of 1-benzothiophene and hydrogenation (o-HYD) of 1-methylcyclohex-1-ene. They were isolated by combination of chromatographic techniques and were undoubtedly assigned

via NMR spectroscopy. The collected 1H NMR data of individual dimethyl-cyclopentenes and ethylcyclopentenes ensures more accurate NMR prediction of cyclopentene derivatives and other related compounds in the future. The identification of the minor volatile content was found to be the crucial step in forthcoming kinetic study of the hydrogenation process. [Refs. 22, 23, 24]



Model hydrotreaning reactions for unconventional catalysts

Microalgaes as a promising source of omega-3 unsaturated fatty acids and their incorporation into the human food chain

(F. Kaštánek, kastanek@icpf.cas.cz; joint project with Rabbit Trhový Štěpánov a.s., IBOT, EcoFuel Laboratories, Institute of Microbiology CAS, Mydlářka a.s., Rabbit CZ a.s., Rabbit Chotýšany a.s., CU, ICPF, UCT Prague; supported by TACR, project No. TA03011027)

The project is focused on utilization of the lipid new sources with the high content of the healthy polyunsaturated fatty acids (PUFAs), omega-3 types. Microorganisms, mainly bio-technologically produced eustigmatofit microalgaes with the high content of PUFA, have been applied. New types of mixotrophic bioreactors were designed to obtain the optimal content PUFA in biomass. Products will be used as the feeding additives for poultry.

The newly designed mixotrophyreactor

Innovative autoMotive MEA Development - implementation of Iphe-genie Achievements Targeted at Excellence (IMMEDIATE)

(L. Kaluža, kaluza@icpf.cas.cz; supported by European Union´s 7th Framework Programme FP7/2007-2013 for the Fuel Cells and Hydrogen Joint Undertaking Technology Initiative, project No. 303466 and co-supported by MEYS, project No. 7HX13003)

Catalysts consisting of 60 wt.% of Pt were prepared by one-step impregnation of the studied high-surface-area carbon black ENSACO® 350G using PtO_2, H_2PtCl_6, $Pt(C_5H_7O_2)_2$, $Pt(NH_3)_4(NO_3)_2$, and $Pt(NH_3)_2(NO_2)_2$ solutions or slurries. These deposited species were reduced to metallic Pt at 0, 70, 120, 140, and 150 °C, respectively. Calcination in Ar followed by reduction in an H_2/Ar mixture at 190 °C ranked these catalysts in the following order of increasing Pt particle size: 3 < 8 < 11-17 ~ 16 < 18-35 nm for the precursor H_2PtCl_6, $Pt(NH_3)_2(NO_2)_2$, $Pt(C_5H_7O_2)_2$, $Pt(NH_3)_4(NO_3)_2$, PtO_2, respectively, favoring H_2PtCl_6. A dechlorination procedure based on one extraction with NaOH solution followed by intensive rinsing with distilled water was developed to decrease the level of hydrolyzable chloride well below 100 ppm in the H_2PtCl_6 based catalyst. The dechlorination increased the Pt particle size from 3 to 4.5 nm.

An experimental carbon black ExpCB of intermediate surface area 384 m^2g^{-1} was compared with the 350G of 808 m^2g^{-1} and with the low surface area carbon blacks 290G and XC72 of 226 $m^2g^{-1}$and 236 m^2g^{-1}, respectively. Laser Raman spectroscopy revealed that all supports contained turbostratic graphitic crystallites of similar size of about 5 nm. Deposition

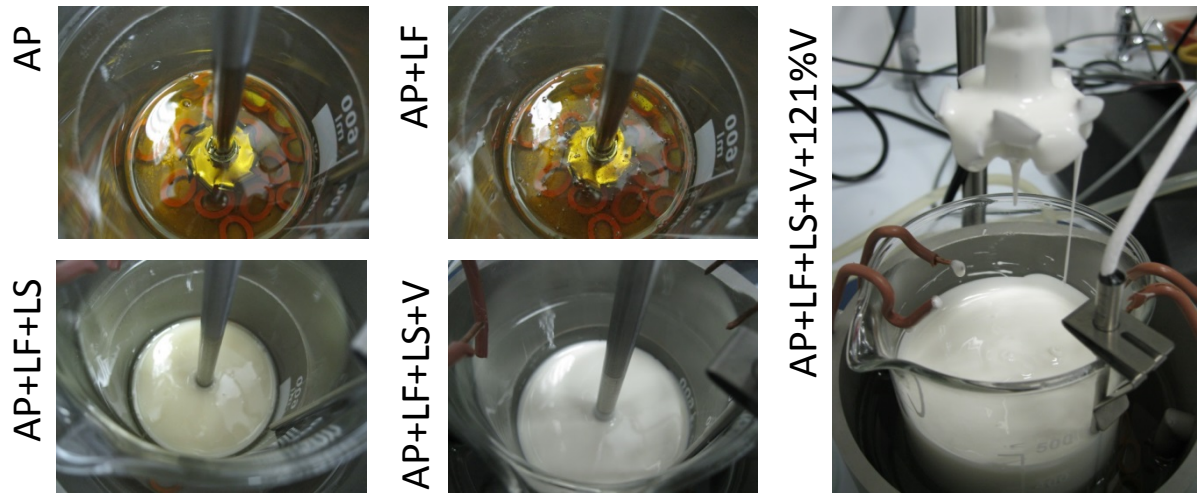
of 60 wt. % Pt on ExpCB by impregnation with H_2PtCl_6 resulted in Pt particle sizes of 4.7 and 8.3 nm for non-dechlorinated and dechlorinated catalyst, respectively. XRD analysis practically confirmed the Pt particle size found by hydrogen pulse chemisorption in the dechlorinated H_2PtCl_6/ExpCB(CRNaWR) catalyst, rendering the value of 10 nm.

Electrochemical RDE analysis indicated that impregnation by H_2PtCl_6 is the most suitable of the catalyst synthesis methods applied in this study. Mass-specific ORR activities in the same order as that for the commercial reference catalyst are obtained for catalysts prepared this way. Due to better electrochemical stability the carbon ExpCB was found to be a better suited catalyst support material than 350G. The electrochemical measurements also indicated that further increase in stability is achieved by dechlorinating the catalyst according to the procedure developed in this study.

Research and development of special dyes using ionic liquids as efficient functional additives

(P. Klusoň, kluson@icpf.cas.cz; joint project with Teluria, Techem; supported by MIT, project No. FR-TI3/057)

This project deals with utilization of special types of ionic liquids based on tetra-alkyl ammonium bistriflateamides as additives for new types of dyes. These additives may bring special properties to the final product, such as higher mechanical stability, higher effect of the pigment addition and lower amounts of various pigments, more complex compositional solutions, etc. The project comprises preparation of the selected ionic liquids, their characterization by many types of physical methods (viscosity, contact angle, density, etc.), and then their direct application together with other characteristic components. The project addresses completely new way to obtain modern dyes useful both in industry as well as for standard and common customers.



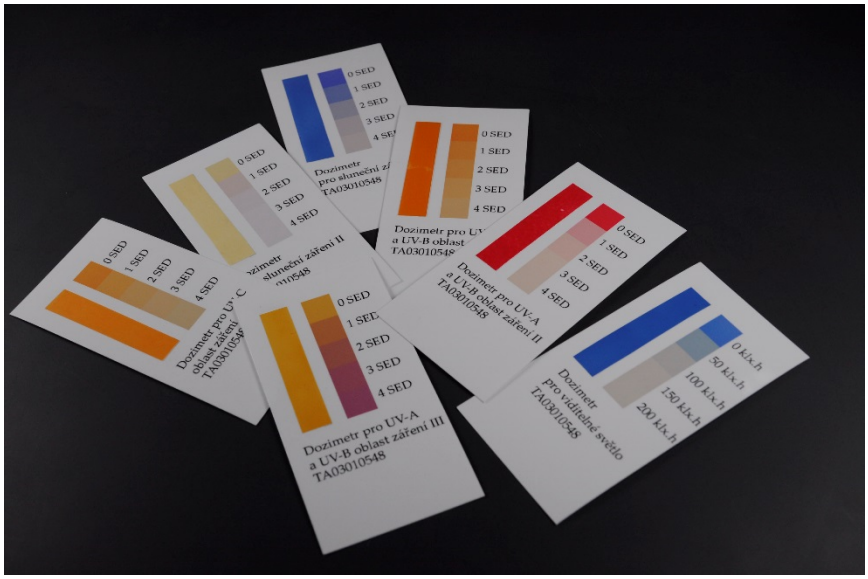
Emulsification progress with and without special additives

Research and development of advanced thin film elements for direct evaluation of the time variable with by means of the preciously calibrated color change

(P. Klusoň, kluson@icpf.cas.cz; joint project with INVOS Ltd., COC Ltd., CU, ICPF, TU Brno; supported by TACR, project No. TA03010548)

Aim of the project, shortly named *Color Clocks,* focuses on the applied research & development and testing of the advanced thin film elements for direct evaluation of the time variable by means of preciously calibrated color change. These elements represent a highly specific form for time measurement under highly specific conditions and for very specific

practical purposes. These structures are supposed to be used as tools for simple visual and intuitive evaluation of the time variable under very different circumstances. It is a kind of standard memory element collecting a certain type of data, which are then assessed in the cumulative form as the absorbed light dose of characteristic energy, or characteristic energetic region. The light sensitive films are based on uniformly organized nanoparticles that exhibit an adjustable photocatalytic activity toward the decomposition of selected organic structures deposited onto their surfaces. The decolorization process is then carefully calibrated for many different types of probe organic molecules. There are many possible practical applications of these materials, among others dermatology, conservation and storage of historical monuments and artefacts, should be mentioned. [Refs. 3, 4, 8]



UV-light exposition sensors

Use of PFG NMR, stochastic reconstruction and molecular simulation to estimate transport-related texture characteristics of advanced porous materials

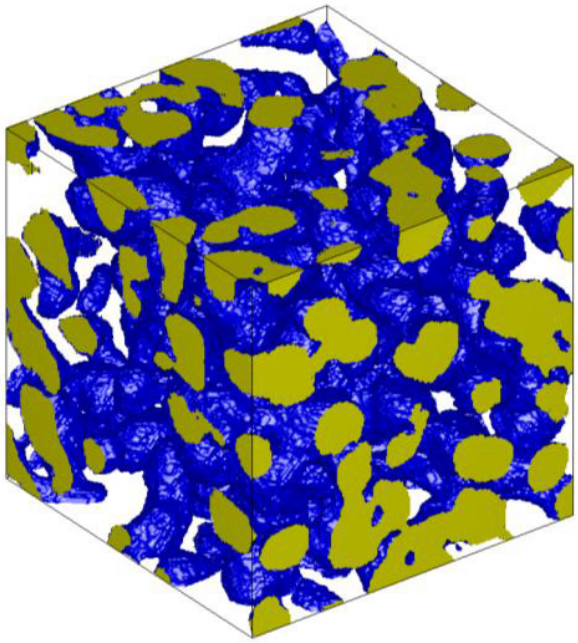
(O. Šolcová, solcova@icpf.cas.cz; joint project with CU and JH IPC; supported by GACR, project No. P204/11/1206)

Microstructures of three mixed-matrix membrane samples made of polyimide and silicalite-1 particles were reconstructed using a stochastic reconstruction procedure. The results of this reconstruction were tested by simulating the random walk of CO_2 molecules in the reconstructed bodies and by predicting the effective permeability of CO_2. Both original and reconstructed membranes revealed a similar enhanced effective permeability, which exceeded predictions based on the effective medium approximations. Therefore, it was suggested that clustering of the silicalite-1 particles was the primary cause of the permeability increase.

The sensitivity analysis of gas transport problems related to experimental setups that are routinely used for determination of effective transport parameters of macroporous solids is presented. The relevance of large total pressure variations to reliable estimation of the effective transport parameters is emphasized in two experimental setups, particularly quasistationary permeation and classical Wicke–Kallenbach cells.

The effective transport properties of advanced porous materials based on hydroxyapatite nanopowders were characterized by means of the effective diffusion coefficients. Polystyrene molecules substituted a role of biofluids transported in human body (especially in bones) were used as appropriate model compounds. The effective diffusion coefficients for two

polystyrene samples with different relative molecular weights (1000 and 100,000) in cyclohexane on hydroxyapatite were evaluated. It was found that the binary effective diffusion coefficients revealed much lower values in comparison with the binary bulk ones due to the strong influence of hindered diffusion in hydroxyapatite pore network. [Refs.1, 2, 16, 17]



3D replica of mixed matrix membrane M5. The cube size is limited to 200×200×200 voxels for a clear view. The phase interface is blue. Intersections of silicalite particles and cube walls are yellow. The polyimide phase is transparent

Removal of endocrine disruptors from waste and drinking water by photocatalytic and biological processes

(O. Šolcová, solcova@icpf.cas.cz; joint project with Dekonta, a.s. and Institute of Microbiology CAS; supported by TACR, project No. TA01020804)

Endocrine disruptors represent the group of chemical substances disrupting the hormonal indication of vertebrates and thereby they could encroach on the organism function. To the group of endocrine disruptors belong surfactants, softeners, fungicides, insecticides and some kinds of medications and hormonal contraception. They are commonly presented not only in the waste water but also in the natural water. Endocrine disruptors are persistent to degradation by common chemicals as well as biological and photolytic processes. The necessity of finding the alternative solutions leads to development and use of the new technologies. Photo-catalysis using semiconductor particles have found increasing interest to solve the endocrine disruptors remove problems.

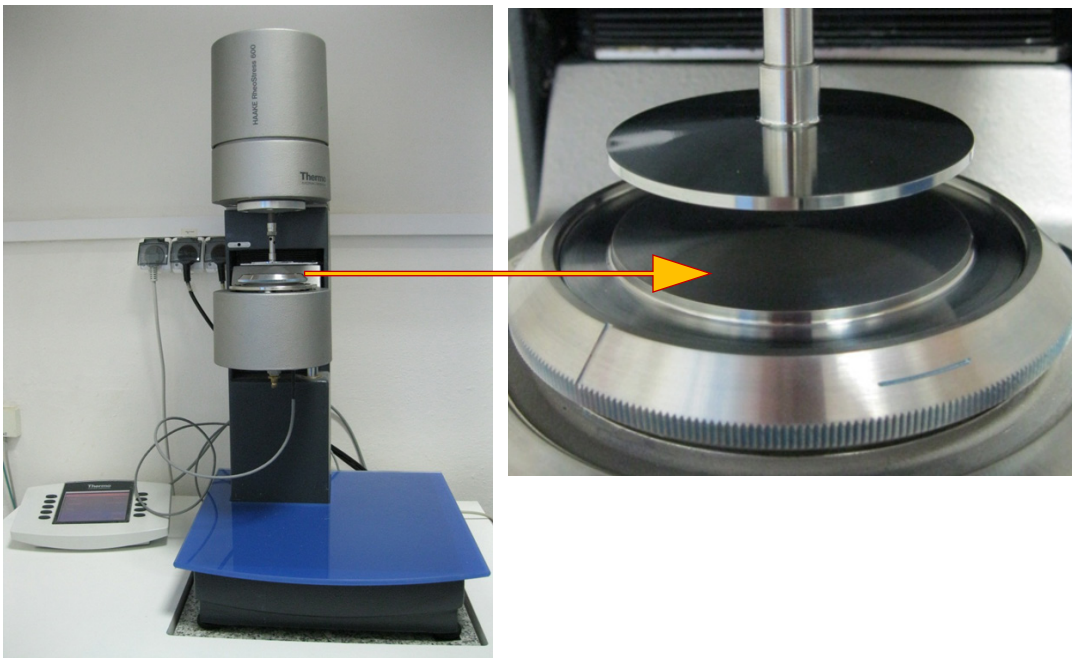
This project is focused on verification of the specially designed photoactive materials and their modified versions suitable for photo-processes carried out upon illumination in the UV-light. Ethynylestradiol, nonylphenol and bisphenol A were chosen as typical compounds belong to the endocrine disruptor group. In this work the water decontamination with various concentrations of endocrine disruptors in the two types of reactors; batch and plug flow arrangement on the titania thin layers were successfully studied. Moreover, the application of the specially designed pilot plan photoreactor was verified on real waste water. [Refs. 9, 10, 25, 27]

Operational tests on sewage plant

Ionic liquids as additives for special pigments

(O. Šolcová, solcova@icpf.cas.cz; joint project with Synthesia, a.s., TECHEM CZ, s.r.o.;
supported by MIT, project No. FR-TI4/189)

Ionic liquids are composed of large ions with a low degree of the overall molecular symmetry. Very high coulombic interactions are behind their impressive electrical and mechanical stabilities, thermal and pressure resistivity, and extremely low tension of vapors. Low flammability, very good electrical conductivity, high thermal capacity and unusual phase behavior might be added to the previous list of exceptional properties. No doubts these features qualify them for a broad band applications ranging from "green solvents" due to their negligible volatility, over templates for synthesis of nanoparticles (some of them tend to form organized ionic clusters), liquid electrolytes in solar cells and fuel cells, to liquid adhesives, special lubricants, chromatography mobile phases, incombustion additives, etc. One of the most prominent applications is their use as special additives for pigments and dye compositions. If the side-chains are too short, they do not disturb the ionic network significantly and, also, they do not possess enough conformational freedom to adopt a low energy configuration. However, increasing the chain-length the role of its spatial arrangement becomes much more important. In this respect this project pays special attention to the utilization of quaternary ammonium ionic liquids, namely n-alkyl-triethyl ammonium bis(trifluoromethane sulfonyl) imides ($N_{R222}Tf_2N$, R = 6, 7, 8, 10, 12, 14) with a variable length of an alkyl chain are specially promising.



Applied rheometer Haake RS 600 a detail of sensor panel

New heterogeneous catalysts for environmental protection

(L. Kaluža, kaluza@icpf.cas.cz; joint bilateral co-operation with Institute of Catalysis, BAS, Sofia, Bulgaria; supported by CAS)

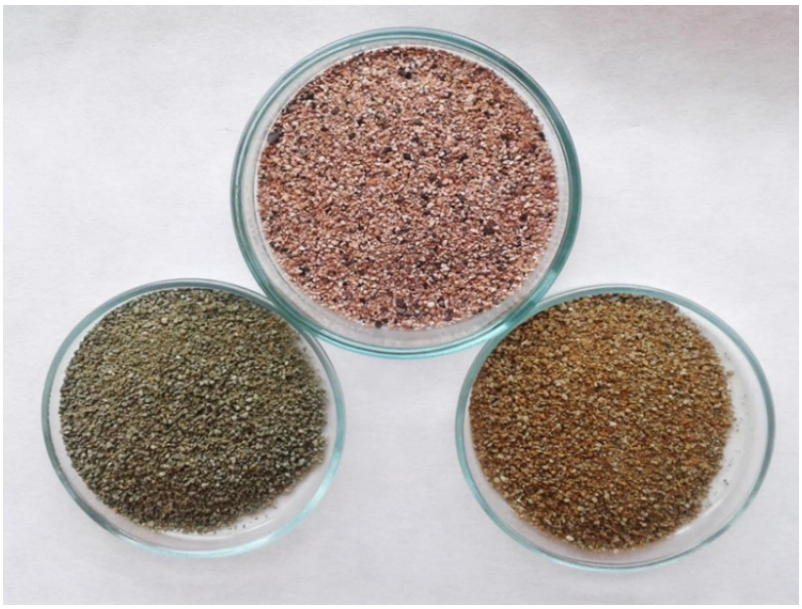
High surface area TiO_2 nanotubes (Ti-NT) synthesized by alkali hydrothermal method were used as a support for NiW hydrodesulphurization catalyst. Nickel salt of 12-tungstophosphoric acid ($Ni_{3/2}PW_{12}O_{40}$) was applied as oxide precursor of the active components. A polytungstate phase evidenced by Raman spectroscopy was observed indicating the destruction of the initial heteropolyanion. The catalytic experiments revealed two times higher thiophene conversion on NiW catalyst supported on Ti-NT than those of catalysts supported on alumina and titania. Increased HDS activity of the NiW catalyst supported on Ti-NT could be related to a higher amount of W oxysulfide entities interacting with Ni sulfide particles as consequence of the electronic effects of the Ti-NT observed with XPS analysis.

Enhancement of the power transformer operation security and prevention of their failures caused by the corrosive sulphur effect

(O. Šolcová, solcova@icpf.cas.cz; joint project with Orgrez, a.s.; supported by TACR, project No. TA04020151)

Recently, a significant volume of research has been undertaken in order to understand the failure of relatively new oil-filled transformers. The cause of failure has been a short circuit in the dielectric isolation. This effect is attributed to the so-called “corrosive sulphur”. Corrosive sulphur is defined as various forms of organic sulphur compounds (often thermally unstable) such as Cu_2S, which can cause corrosion of metal parts of the transformer, in particular copper and silver. Dibenzyl disulfide has been found to be the leading corrosive sulphur compound in the insulation oil. This project is focused on finding an effective way to decontaminate such oils. Commonly used transformer oils were purified by sorption technique and by extraction into polar aprotic solvents such as acrylonitrile, dimethyl sulfoxide, N-methyl-2-pyrrolidone or dimethylformamide. The key physico-chemical and chemical properties of transformer oils containing corrosive sulphur were defined. Therefore,

viscosity at 40°C, density at 20°C, contact angle, group composed of transformer oils, distillation curve by simulated distillation, content of sulphur compounds in the oil samples by mass spectrometry (GC/HRMS) and gas chromatograph with chemiluminescence sulphur detector (GC SCD) were determined.



Tested natural sorbents

Decontamination of brownfields extensively contaminated by organic compounds and heavy metals

(O. Šolcová, solcova@icpf.cas.cz; joint project with Dekonta, a.s.; supported by TACR, project No. TA04020700)

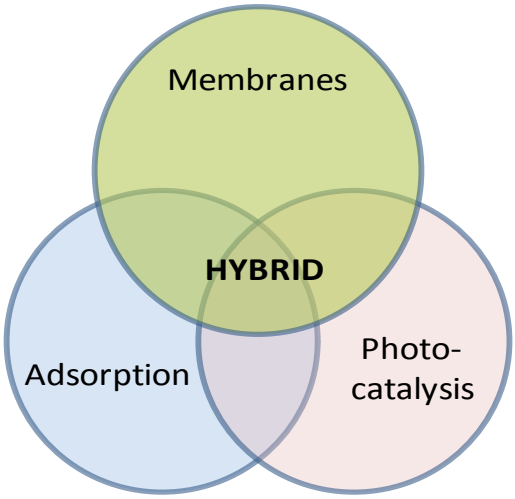
This project is aimed at finding an optimized solution for soil and groundwater treatment at various brownfield sites. During this project, methods enabling decontamination of premises polluted by a broad range of contaminants, such as petroleum substances, polyaromatic hydrocarbons, or chlorinated and polychlorinated persistent organic pollutants, and heavy metals, will be verified. These techniques will be based on optimized combining of selected physical-chemical processes. Emphases will be put on a treatment train application, comprising adsorption, thermic desorption in aerobic and inert conditions, catalytic incineration, reductive dechlorination, chemical solidification of heavy metals as well as advanced oxidation of water including photocatalytic treatment. Efficiency and economic feasibility of laboratory designed and experimentally tested means of decontamination will be further proven on semipilot and pilot-scale model systems. Technological conclusions will be evaluated on processing of soil from selected brownfields and other contaminated sites in the Czech Republic. Novelty of the proposed project lies in elaboration of a method for separating of heavy metals from gas phase produced during thermal desorption and an algorithm of precisely defined subsequent decontamination methods, which will be verified in practice. The developed algorithm will cover majority of possible pollutant's combinations occurring in brownfields. In the Czech Republic, the problem of brownfields' decontamination in such scope as well as such a comprehensive way has not yet been dealt. [Refs. 7, 11, 20, 28]

Laboratory reactor for thermal desorption

Hybride membrane process for water treatment (HYMEPRO)

(O. Šolcová, L. Matějová (member of the steering group), solcova@icpf.cas.cz, matejova@icpf.cas.cz; joint project with University of Oulu, Lappeenranta University of Technology, Corvinus University of Budapest, National University of Engineering in Lima and 12 industrial partners; supported by Finish funding agency TEKES)

Project deals with the development of a novel, active and sustainable hybrid wastewater treatment process that removes simultaneously heavy metals, arsenic and nutrients from waters. The developed technology is designed based on the green chemistry and engineering principles. [Refs. 13, 21]



Production of 3rd generation biofuels by enzymatic catalyzed transesterification of microalgal oil

(O. Šolcová, solcova@icpf.cas.cz; joint project with EcoFuel Laboratories, TransBiodiesel, Ltd. Israel; supported by MEYS, GESHER/MOST, project No. LJ12002)

The objective of the project is to develop a closed process for autotrophic cultivation of microalgae and biorefinery approach using novel extraction techniques for production of algal

oils and high-value feed additives from wet algal biomass. The oil will be further converted to biodiesel utilizing a novel immobilized enzymatic technology.

Project makes huge benefit from connecting algae cultivation and photo-bioreactor design experience together with the down-stream chemical engineering experience of Czech partners with the complementary experience of Israel partner in the area of biodiesel production. Important benefit lies in the transfer of developed algal biotechnologies to Israel where conditions of warm Mediterranean climate with high level of photosynthetic solar radiation will allow efficient year-round large-scale cultivation of algae mainly using deserted non-arable land for photobioreactors installation. In comparison, climatic conditions in Czech Republic allows for only approx. 150 days cultivation period.

The process consists of cultivation of microalgae in the novel high-rate photobioreactors using waste streams as nutrients, the novel low-energy cell harvesting techniques and lipids extraction directly from wet biomass coupled with advanced high-yield enzymatic transesterification of algal oil into biodiesel. The extraction of oil from algal biomass will be environmentally friendly, leaving residual algal biomass with high content of proteins and carotenoids, suitable for use as animal feed supplement. This biorefinery approach influences positively the feasibility of production of algal biodiesel.

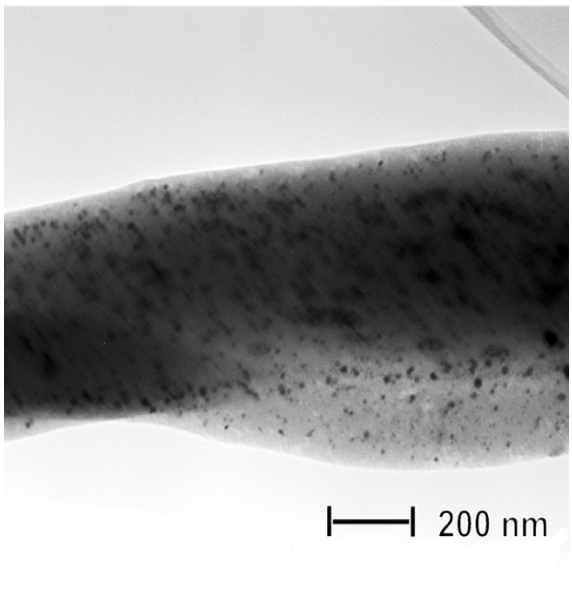
Utilization of vast knowledge of microalgae cultivation techniques and photo-bioreactor existing by partners in Czech Republic will facilitate development of techniques for production of biodiesel feedstock from algal oil. In Israel - TransBiodiesel will contribute to development of non-lipid high tolerance enzymes. Such technologically advanced enzymes will be used in a "pilot unit" for transesterification algal oil using environmentally friendly and energy saving advanced enzymatic process for 3rd generation of biodiesel production.

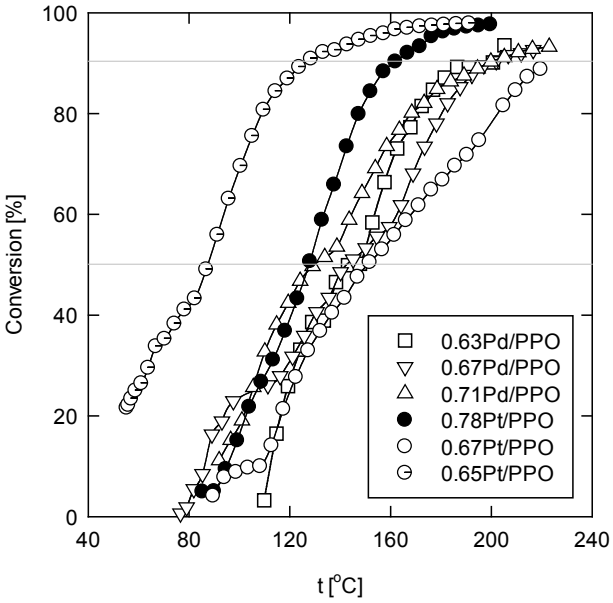
Pilot plant bioreactor

Washcoated ceramic monoliths for total oxidation of volatile organic compounds

(P. Topka, topka@icpf.cas.cz; supported by GACR, project No. 13-24186P)

The effect of impregnation method on the size of palladium and platinum nanoparticles supported on poly(2,6-dimethyl-1,4-phenylene) oxide electrospun mats was investigated. Catalysts with similar metal loading (0.63-0.78 wt. %) possessing various mean metal particle size (2.5 – 8.7 nm) were prepared employing different impregnation times and nominal metal loadings. The catalysts were tested in the total oxidation of methanol (1 000 ppm in air). The catalytic performance of platinum catalysts increased with increasing mean size of Pt nanoparticles. On the other hand, the catalytic performance of palladium catalysts did not correlate with the mean nanoparticle size.





Catalytic performance of platinum and palladium nanoparticles supported on poly(2,6-dimethyl-1,4-phenylene) oxide electrospun mats in the oxidation of methanol

International co-operations

Université catholique de Louvain, Louvain-La-Neuve, Belgium: Chlorobenzene oxidation over platinum and gold catalysts
University of Udine, Udine, Italy: Oxidation of model volatile organic compounds over silver, copper and cobalt catalysts
Institute of Catalysis, BAS, Sofia, Bulgaria: New heterogeneous catalysts for environmental protection
University of Liverpool: Theory of chemical bond
Max-Planck Institute for Chemical Physics of Solids, Dresden: Chemcal bonding in solids
University of Oulu, Oulu, Finland: New catalysts for VOC oxidation
University of Oulu, Oulu, Finland: Hybrid membrane process for water treatment
University of Poitiers, Poitiers, France: New catalysts for VOC elimination
University of Strasbourg, Strasbourg, France: Determination of transport characteristics of novel materials with hierarchical pore structure
University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
University of Maribor, Maribor, Slovenia: PolyHYPE polymers
University of Graz, Graz, Austria: Porous polymers
Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
University of Barcelona, Barcelona, Spain: Ion exchanger catalysts
Zhejiang University, Hangzhou, China: Mesoporous poly(divinylbenzenes)
Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials
University of Bangor, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials

UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification
University of Udine, Udine, Italy: Characterization of noble metal catalysts and desulfurization on unconventional catalysts
Istanbul Technical University, Istanbul, Turkey: Synthesis and Thorough Characterization of Composite Functionalized Polymeric Nano-Structure
Institute of Computational Chemistry, University of Girona, Spain: Computation
IRD Fuel Cells A/S, Svendborg, Denmark: Fuel cells electroactivity
Centre National de la Recherche Scientifique, Montpellier, France: Non-carbonaceous supports, catalysts
FUMA-TECH Gesellschaft für Funktionelle Membranen und Anlagentechnologie MBH, St Ingbert, Germany: Ionomers
Shanghai Jiao Tong University, Shanghai, China: Ionomers and polymers
Volvo Technology AB, Göteborg, Sweden: MAE test protocols
SGL Carbon Gmbh, Meitingen, Germany: Electroconductive gas diffusive layers
JRC Joint Research Centre-European Commission, Brussels, Belgium: FCH tests
TimCal SA, Bodio, Switzerland: Carbon black supports

Visitors

A. Spojakina, Institute of Catalysis, BAS, Sofia, Bulgaria
Dr. Gerardo Cruz, National University of Tumbes, Peru
Dr. Mónica Gómez, National University of Engineering, Lima, Peru
L. Benoit, University of Strasbourg, France
P. Losch, University of Strasbourg, France
J. Grabowski, Central Mining Institute, Katowice, Poland
A. Sezai Sarac, Istanbul Technical University Faculty of Sciences
R. Palcheva, Institute of Catalysis, BAS, Sofia, Bulgaria
K. Stanczyk, Central Mining Institute, Katowice, Poland
Y. Zub, Institute of Surface Chemistry NAS, Ukraine
H. Gao, Shanghai Jiao Tong University, Shanghai, China
B. Bauer, FUMA-TECH, St Ingbert, Germany
W. Zhang, FUMA-TECH, St Ingbert, Germany
D. Jones, Centre National de la Recherché Scientifique, Montpellier, France
J. Roziere, Centre National de la Recherché Scientifique, Montpellier, France
J.L. Bonde, IRD Fuel Cells A/S, Svendborg, Denmark
M. Odgaard, IRD Fuel Cells A/S, Svendborg, Denmark
M.J. Larsen, IRD Fuel Cells A/S, Svendborg, Denmark
D.N. Tito, Elysium Projects Ltd., Bangor, United Kingdom
John Bostock, Elysium Projects Ltd., Bangor, United Kingdom

Teaching

P. Krystyník: UJEP, Faculty of the Environment, course "Toxicology"
R. Ponec: CU, Faculty of Science, course "Physical Organic Chemistry"
O. Šolcová: UCT, Prague, Faculty of Chemical Technology, postgraduate course "Texture of Porous Solids"

Publications

Original papers

[1] Čapek P., Veselý M., Bernauer B., Sysel P., Hejtmánek V., Kočiřík M., Brabec L., Prokopová O.: Stochastic Reconstruction of Mixed-Matrix Membranes and Evaluation of Effective Permeability. *Comput. Mat. Sci.* 89, 142-156 (2014).

[2] Čapek P., Veselý M., Hejtmánek V.: On the Measurement of Transport Parameters of Porous Solids in Permeation and Wicke-Kallenbach Cells. *Chem. Eng. Sci.* 118, 192-207 (2014).

[3] Dytrych P., Klusoň P., Dzik M., Veselý M., Morozová M., Sedláková Z., Šolcová O.: Photo-Electrochemical Properties of ZnO and TiO_2 Layers in Ionic Liquids Environment. *Catal. Today* 230, 152-157 (2014).

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[26] Ponec R.: Late Reminiscence of Unexplored Scientific Links with Ante. Parity of Kekulé Structures and Algebraic Structure Count. In: *Ante Graovac - Life and Works*. (Gutman, I.- Pokric, B.- Vukicevic, D., Ed.), pp. 243-258, University of Kragujevac, Kragujevac 2014.

Patents

[27] Kaštánek F., Šolcová O., Maléterová Y., Spáčilová L., Maternová H., Mašín P., Žebrák R: Zařízení pro fotokatalytickou dekontaminaci vod s obsahem organických látek, zejména endokrinních disruptorů. Device for Photo-Catalytic Decontamination of Water Containing Organic Compounds, Especially Endocrine Disruptors. *Pat. No. 304681*/PV 2013-522. Applied: 13.07.03, Patented: 14.07.17.

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Department of Multiphase Reactors

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PHD STUDENTS
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LAB TECHNICIANS
DAVID KARFÍK

Fields of research

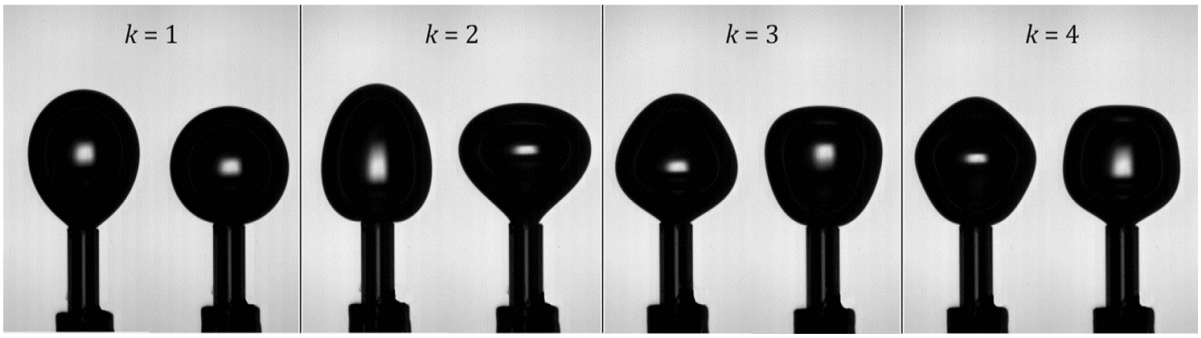
- Fluid dynamics and transport phenomena in multiphase systems of gas-liquid, liquid-solid or gas-liquid-solid type
- Influence of surface active agents on the multiphase flows
- Powder rheology, sedimentation of granular mixtures or complex assemblages
- Numerical simulations of the gas-liquid and granular systems (with Fluent, CFX, DEM)
- Flow of a liquid or gas-liquid dispersions in channels or microchannels
- Electrodiffusion diagnostics of the flow
- Hydroacoustic detection of bubbles using sonar in shallow reservoirs
- Complex rheological behavior of microdispersions
- Stability and behaviour of complex beverage foams

Research projects

Effect of surfactants on the multiphase flow dynamics

(J. Vejražka, vejrazka@icpf.cas.cz; supported by GACR, project No. P101/11/0806)

The effect of surface-active agents on two-phase flows is studied. Flow types "air bubbles in the liquid" and "liquid drops in another immiscible liquid" are focused. Some specific situations, in which the surfactants modify the flow at the bubble/drop scale and in which this modification cannot be explained by a simple change of the equilibrium surface tension, are investigated experimentally. These situations are (i) the shape oscillations of a bubble/drop, both freely-rising or attached at a capillary tip; focus is put on the modification of oscillation frequency and decay time by surfactants; (ii) the coalescence of bubbles/drops, and also their attachment to a solid surface, with a focus on the drainage of liquid film between them; (iii) the bubble-solid surface collision, with a focus on suppression of the bubble rebound caused by surfactants and also on the modification of the attachment time; (iv) break-up of bubbles in a turbulent flow. The research should enlighten and document the effect of interfacial properties other than surface tension on two-phase flows. [Ref. 8]

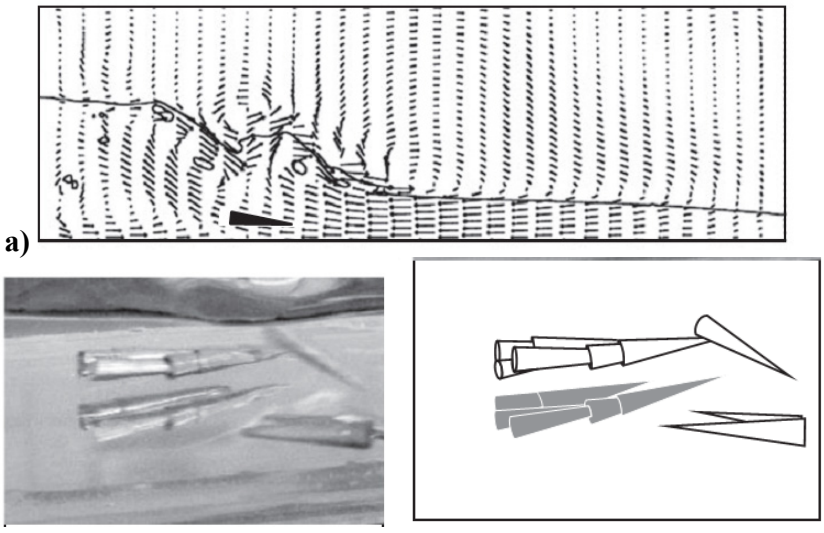


Shape of first four eigenmodes of an oscillating 1mm bubble at a small capillary

Hydrodynamic experiments on dacryoconarid shell telescoping

(M. Růžička, ruzicka@icpf.cas.cz; joint research with Institute of Geology CAS)

It is not uncommon that small conical dacryoconarid shells are found inserted one into another, however, no satisfactory explanation has been provided. We performed experiments under laboratory conditions using narrow aluminum cones as replicas of these shells. Two different flow regimes were tested to mimic the probable hydrodynamic conditions in the ocean. First, large-scale rhythmic back and forth coherent motion of water over the seabed was reproduced in an oscillating sloshing tank (sloshing mode). Second, small scale irregular stirring motion in turbulent bulk was imitated in cylindrical containers placed into a shaker (mixing mode). With sloshing, a high production of irreversibly telescoped cones was present in clear water and at driving frequencies comparable to the upper limits known for sea waves. With shaking, both coalescence and break-up of the cones were observed, as the quasi-random hydrodynamic forces generated by vigorous liquid motion were roughly comparable with the mechanical forces holding the cones together. In addition, a simple mathematical model was suggested for the flow interaction with a submerged conical particle in the case of the sloshing mode, providing an interesting insight into the evolution of strong deceleration zones. [Ref. 3]

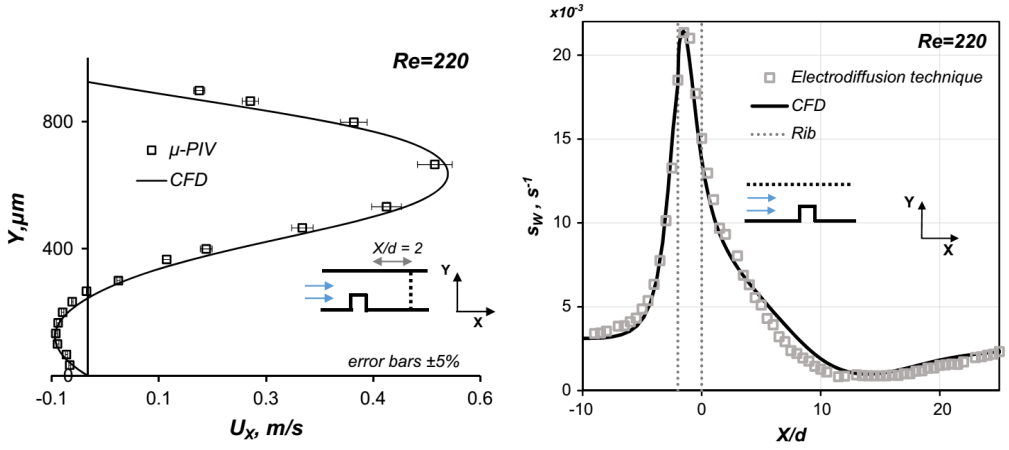


Experimental and numerical evaluation of the origin of conical shell concentrates:
a) Numerical simulation of particle motion in a sloshing tank,
b) Photos of shells and redrawn picture illustrating moment of telescoping

Application of the electrodiffusion sensors to the flow diagnostics in microfluidic systems

(J. Tihon, tihon@icpf.cas.cz; supported by GACR, project No. P101/12/0585)

The project is focused on characterization of two-phase flows in microfluidic systems. The high-tech fabrication techniques will be used to produce microdevices with precisely located microelectrodes. These electrodiffusion sensors for the near-wall flow diagnostics will be, for the first time, implemented at a microfluidic scale. The proposed measurements will provide information on the wall shear stress, the local flow structures, and the effect of bubbles/particles on the near-wall flow region (e.g. the liquid film under bubbles, the apparent wall slip in microdispersions). The application of the particle image velocimetry together with the microscopic visualization techniques will complete the hydrodynamic picture of the studied microfluidic flow configurations (junction, crossing, sudden expansion). It is expected that the electrodiffusion method will be proved as a suitable tool for microdevice diagnostics. The obtained experimental knowledge and the derived physical models will be useful for design, control, and optimization of microfluidic devices. [Refs. 1, 5, 7]

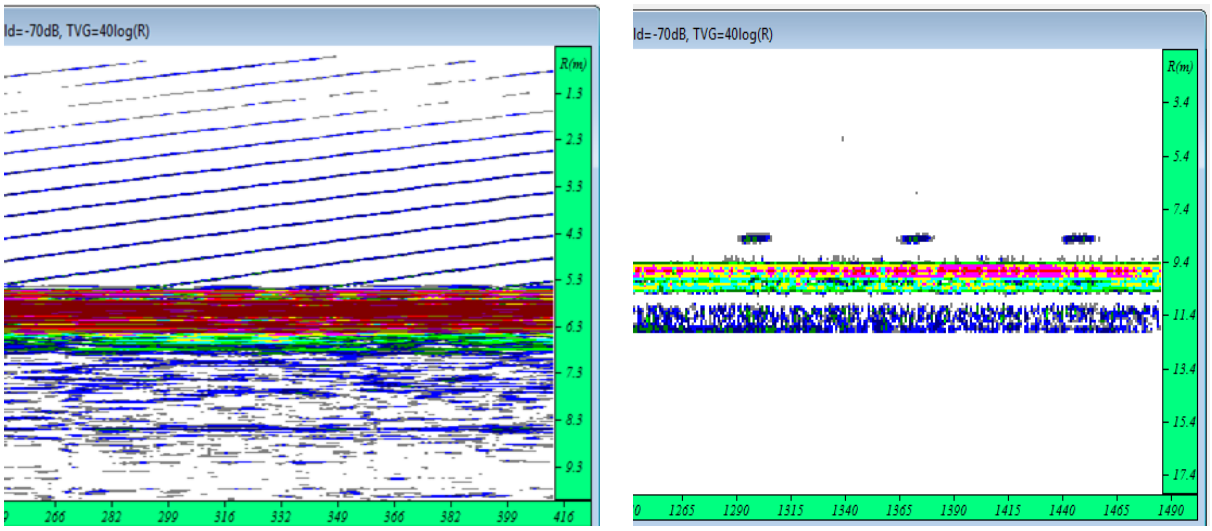


Velocity profile reconstruction from μ-PIV for laminar region (left) and corresponding shear rate on the wall above the rib along the X-axis using the electrodiffusion technique (right). Both measurements was compared with CFD simulation

Hydroacoustical distinguishing between fish and bubbles, and quantification of methane bubble ebullition in freshwater reservoirs of temperate zone

(P. Stanovský, stanovsky@icpf.cas.cz; joint project with Institute of Hydrobiology and Biology Centre of the CAS; supported by GACR, project No. P504/12/1186)

The acoustic parameters of rising methane bubbles will be measured by echo sounders at different frequencies at man-made bubbles. The special algorithms using multi-frequency record will be developed to distinguish the bubble echoes from the fish echoes having the same acoustic size. The obtained method will be used to estimate of fish abundance and biomass more accurately. Further, the model describing the bubble rise and dissolution in will be modified for freshwater lakes. The relation between bubble volume and acoustic echoes from experiments with man-made bubbles will be used to gain more exact data about the amount of the methane bubbles ebullated from the chosen reservoirs in temperate zone. The spatio-temporal changes in their productions will be monitored also. At the end, the research should enlighten the correlation of the quantity and quality of ebullated methane bubbles with the environmental conditions.

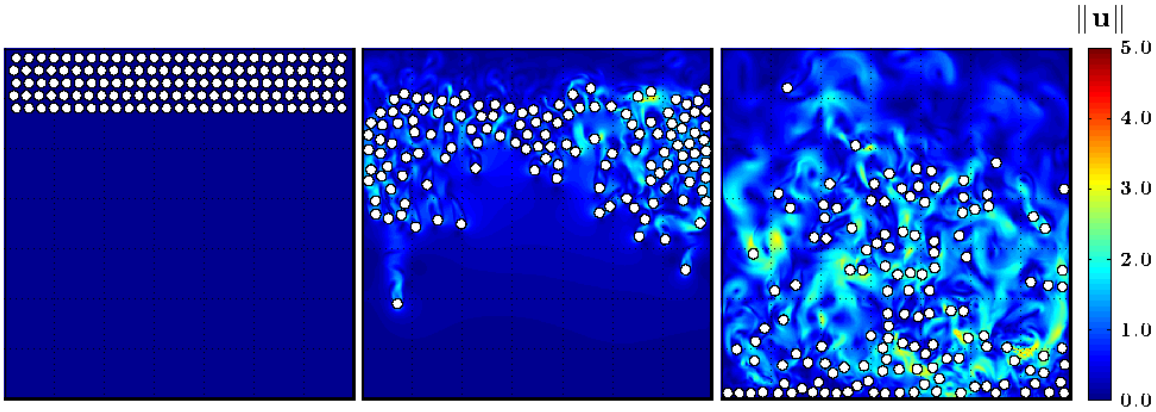


Acoustic echoes of 3 mm bubbles recorded by vertical (left) and horizontal (right) sonar. Blue lines (rep. spots) represent rising bubbles and brown bar at left image represents bottom of the lake (ordinate – water depth, abscissa – time scale in signal pings)

Hydro-mechanical interactions of particles in solid-fluid systems

(J. Havlica, havlica@icpf.cas.cz; joint project with UCT, Prague; supported by GACR, project No. P105/12/0664)

The solid-fluid dispersions are very complicated multiphase systems with a wide range of interactions of different physical nature. The suggested project is focused on specific topic from this field: the hydromechanical interactions between the solid particles (discrete phase) dispersed in a carrying fluid (continuous phase). The typical feature of these dispersions is the presence of two kinds of force interactions: the fluid forces on the dispersed particles and the mechanical forces between the particles at collisions. These interactions have crucial importance for prediction of flow behavior in process apparatuses or for correct design of industrial technologies. The main aim is to develop physical modeling concepts for solid-fluid dispersions. This concept is based on numerical simulations of these systems and benchmark experiments on static and dynamic behavior. We expect that the project brings important original results, which will help to understand flow behavior of multiphase systems.

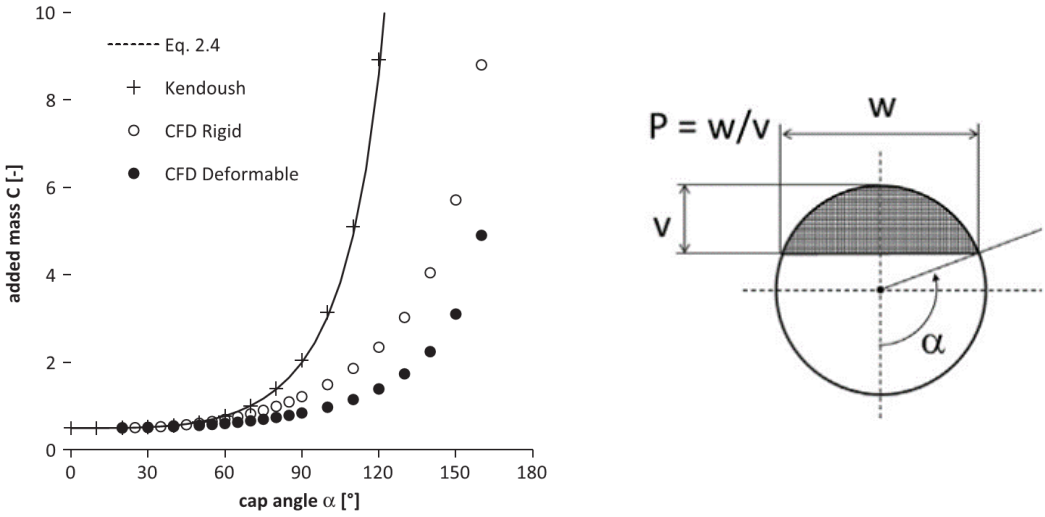


Sedimentation of 135 rigid particles simulated with immersed boundary method

Added mass of spherical cap body in multiphase flow

(M. Šimčík, simcik@icpf.cas.cz; supported by ICPF)

The added mass coefficient *C* was determined for a single spherical-cap body moving in a uniform unbounded fluid. An approximate simple physical model for *C* was suggested and was well compared with the analytical result of Kendoush, which likely is the only available theoretical result in the literature, up to date. The correct result for *C* was obtained via direct numerical flow simulation with CFD. Both the rigid and deformable (bubble, drop) cap body was considered. An approximate model was suggested for the collective added mass in a swarm of spherical cap bodies. A relation was found between the added mass of an unbounded cap body and a bounded spherical body. Practical explicit correlation formulas for *C* were obtained, suitable for engineering modelling of multiphase flow systems with bubbles, drops and solids. A relation between the added mass, Darwin drift, and fluid mixing was also noted. [Ref. 6]



Added mass coefficient C for a spherical-cap body. Kendoush - approximate analytical solution for a rigid cap by *Kendoush* (2003). Blank points- Direct numerical solution by CFD for deformable cap-body. Full points - Direct numerical solution by CFD for rigid cap-body. Equation (2.4) - approximate physical model for a rigid cap.

International co-operations

Institute of Fluid Mechanics, Toulouse, France: Effect of surfactants on multiphase flows
Norwegian Institute of Technology (NTH), SINTEF, Trondheim, Norway: Bubble columns

Centre de Recherché et de Transfert de Technologies, Saint Nazaire, France: Microfluidics
Aristotle University of Thessaloniki, Thessaloniki, Greece: Microfluidics
University of Nottingham, United Kingdom: Multiphase diagnostics in gas-liquid flows
Università degli Studi di Napoli Federico II., Italy: Bubble columns and coalescence

Visitors

L. Muscat, INP ENSEEIHT Toulouse, France

Teaching

J. Drahoš, M. Růžička: UCT, Prague, Faculty of Chemical Engineering, postgraduate course "Multiphase Reactors"
J. Havlica: UJEP, Faculty of Science, courses “Mathematics”, “Chemical Engineering”, "Programming in Chemistry"
J. Tihon, J. Vejražka: UCT, Prague, Faculty of Chemical Engineering, postgraduate course "Bubbles, Drops, and Particles"

Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)

Publications

Original papers

[1] Böhm L., Sepideh J., Tihon J., Bérubé P.R., Kraume M.: Application of the Electrodiffusion Method to Measure Wall Shear Stress: Integrating Theory and Practice. *Chem. Eng. Technol.* 37(6), 938-950 (2014).

[2] Dolejš P., Poštulka V., Sedláková Z., Jandová V., Vejražka J., Esposito E., Jansen J.C., Izák P.: Simultaneous Hydrogen Sulphide and Carbon Dioxide Removal from Biogas by Water-Swollen Reverse Osmosis Membrane. *Sep. Purif. Technol.* 131, 108–116 (2014).

[3] Hladil J., Šimčík M., Růžička M., Kulaviak L., Lisý P.: Hydrodynamic Experiments on Dacryoconarid Shell Telescoping. *Lethaia* 47(3), 376-396 (2014).

[4] Morávková L., Vopička O., Vejražka J., Vychodilová H., Sedláková Z., Friess K., Izák P.: Vapour Permeation and Sorption in Fluoropolymer Gel Membrane Based on Ionic Liquid 1-Ethyl-3-Methylimidazolium bis(trifluoromethylsulfonyl)Imide. *Chem. Pap.* 68(12), 1739-1746 (2014).

[5] Stogiannis I.A., Passos A.D., Mouza A.A., Paras S.V., Pěnkavová V., Tihon J.: Flow Investigation in a Microchannel with a Flow Disturbing Rib. *Chem. Eng. Sci.* 119, 65–76 (2014).

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[7] Tihon J., Pěnkavová V., Vejražka J.: Wall Shear Stress Induced by a Large Bubble Rising in an Inclined Rectangular Channel. *Int. J. Multiphase Flow* 67, 76–87 (2014).

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[9] Wichterle K., Večeř M., Růžička M.: Asymmetric Deformation of Bubble Shape: Cause or Effect of Vortex-Shedding? *Chem. Pap.* 68(1), 74-79 (2014).

Patents

[10] Brányik T., Růžička M., Poštulková M.: Zařízení pro stanovení přepěňování sycených nápojů. Apparatus for Gushing Analysis in Carbonated Beverages. *Pat. No. 26362*/UV 2013-28285. Applied: 13.08.05, Patented: 14.01.20.

[11] Veselý V., Drahoš J., Šírek M.: Process for Recovering Terephthalic Acid. *Pat. No. EP2061744*/PCT/ CZ2007/000086. Applied: 07.09.06, Patented: 14.04.30.

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Fields of research

- Helicene based chiral stationary phase for HPLC
- Chiral separation of helicenes
- Rearrangement of 1-methylcyclohex-1-ene during hydrodesulfurization of FCC gasoline
- Highly fluorous cyclopentadienes for application in catalysis
- Peracetylated 3-deoxy-3-fluoro analogs of D-glucosamine and D-galactosamine
- Synthesis of helicene derivatives and [*n*]phenacene derivatives
- Sensors based on laser ablated graphene
- Silicon nanowires grown on metal substrates

Applied research

- Enzymatic optical sensor and optical fiber biosensor of glucose
- Printed optical chemical sensors
- Development of new analytical methods
- Analytical services to the research departments of ICPF
- Highly efficient catalyst and process for degradation of resistant antibiotics
- Macroporous titanium surfaces for enhancing bone osseointegration and adhesion to titanium implants

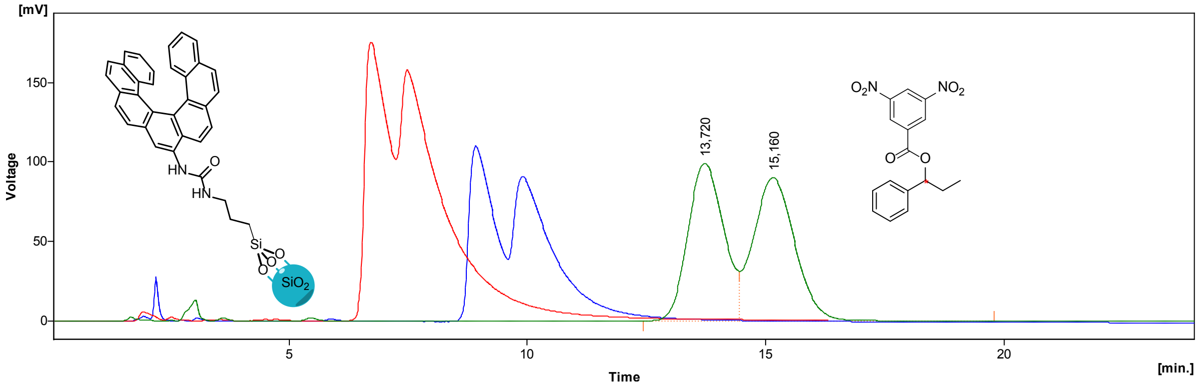
Research projects

Preparation of helicene based chiral stationary phase for HPLC

(J. Sýkora, sykora@icpf.cas.cz; joint project with Watrex Praha, s.r.o.; supported by TACR, project No. TA01010646)

The main aim of the project is to develop a new chiral stationary phase for HPLC which would serve for column manufacturing. During the project the procedure for large scale production of helicene derivatives has been developed and patented. The explored reactivity of 9-bromo[7]helicene was utilized in preparation and subsequent electropolymerization of [7]helicenyl-thiophene. [Ref. 8]

During the fourth year of the project pure enantiomers of 9-amino[7]helicene were isolated, reacted with 3-(triethoxysilyl)propyl isocyanate and finally anchored onto silica. The performance of new chiral stationary phase was then tested on various racemic substrates in order to evaluate the relevancy for possible HPLC column production and sale.



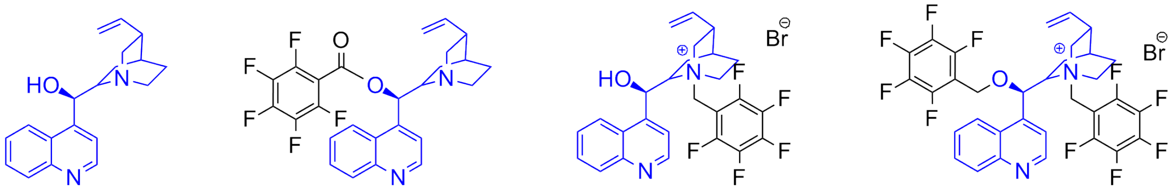
Separation of 1-phenylpropyl ester of dinitrobenzoic acid (red - helicene based phase endcapped, blue - no endcap, green - Kromasil Cellucoat phase), column dimensions 150 x 3 mm, flow 0.5 ml / min, temperature 25°C, UV detection at 254 nm

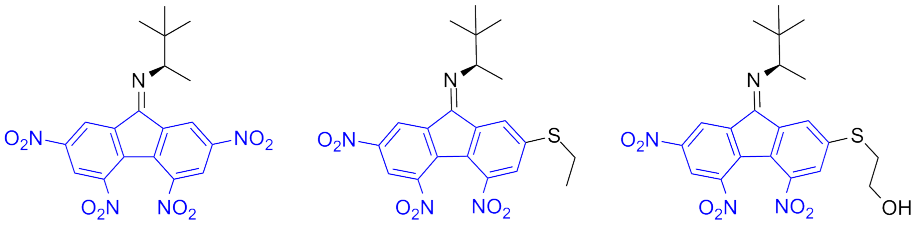
Chiral separation of helicenes

(J. Storch, storchj@icpf.cas.cz; joint project with Lach-ner, s.r.o.; supported by TACR, project No. TA04010082)

The main objective of the project is the development of cheap and effective technology for chiral separation of unsubstituted and substituted helicenes in sufficient quantity enabling further applied research. The sub-objective of the project is to bring new charge-transfer (CT) agents capable of enantiodiscrimination of helicenes. Only optically pure helicenes have the potential to be applied in diverse areas of use such are molecular functional layer (OFET, OLED), liquid crystal display (LCD) and special semiconducting polymers. [Ref. 8]

Within this year we were focused on the synthesis of the electronically deficient cinchonidine and fluorenone CT-agents and complexation studies with various helicenes. Results obtained will be further used for improvement of structures in order to improve enantiodiscrimination abilities and increase stability constant.



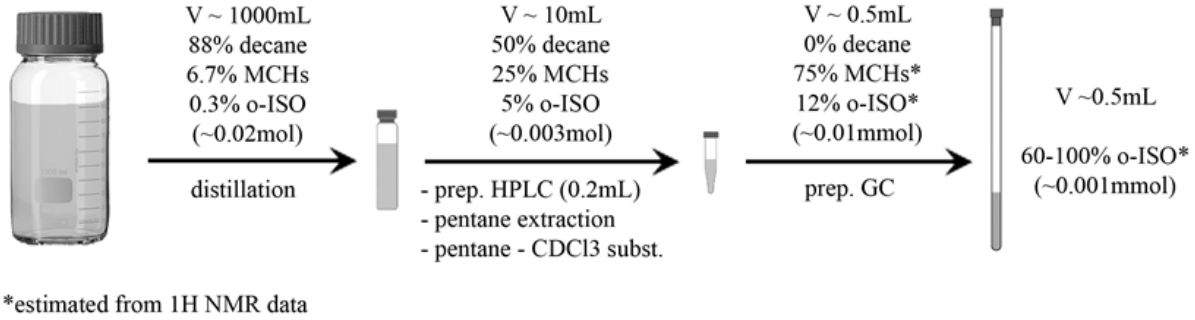


Cinchonidine and fluorenone CT-agents

The rearrangement of 1-methylcyclohex-1-ene during hydrodesulfurization of FCC gasoline over supported Co(Ni)Mo/Al_2O_3 sulfide catalysts: the isolation and identification of branched cyclic C7 olefins

(J. Sýkora, sykora@icpf.cas.cz; project supported by GACR, project No. P106/11/0902)

In the study of simultaneous hydrodesulfurization of 1-benzothiophene and the olefin hydrogenation of 1-methylcyclohex-1-ene we encountered a rearrangement of 1-MCH during the first step of catalytic hydrogenation, which yielded various branched cyclic olefins; mainly ethylcyclopentene and dimethylcyclopentene isomers. The volatile isomerization products were isolated directly from diluted reaction mixture via combination of chromatographic techniques including preparative gas chromatography, and were undoubtedly assigned by NMR spectroscopy. The precise identification of the isomerization products was required for subsequent detail kinetic study. [Ref. 20]



Overview of the isolation procedure

BIO-OPT-XUV Research team advancement at the FBME CTU

(G. Kuncová, kuncova@icpf.cas.cz; supported by MEYS, ESF, project No. CZ.1.07/2.3.00/20.0092)

The project is focused on strengthen education and build up a team at the FBME (Faculty of Biomedical Engineering) CTU. In the academic year 2014/2015, experiments of two Mc. projects of the students of FBME CTU were realized in the laboratory of Immobilized Biocatalyst and Optical Sensors. The topics of these projects were enzymatic optical sensor and optical fiber biosensor of glucose.

Printed Optical Chemical Sensors (POS)

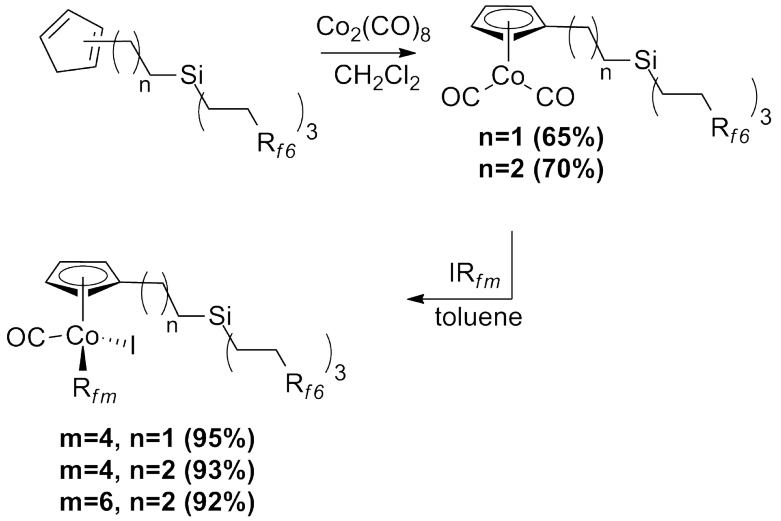
(G. Kuncová, kuncova@icpf.cas.cz; joint project with Invos, s.r.o.; supported by TACR, project No. TA03010544)

Experimental work was focused on the development of optical detector of oxygen. On demand of industrial partner such oxygen detector have to be visible (oxygen is indicated by change of color) printable and cheap. We prepared a series of sensor compositions.

Highly fluorous cyclopentadienes for applications in catalysis

(J. Čermák, cermak@icpf.cas.cz; supported by GACR, project No. P106/12/1372)

Two new fluorous tags based on omega-[tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)-silyl]alkyl substituents (alkyl = ethyl, propyl) synthesized previously were used to prepare cyclopentadienes (the mixtures of 1- and 2-substituted isomers) which bore the tags. Cyclopentadienylcobalt(I) dicarbonyl complexes were subsequently obtained from the reactions of the cyclopentadienes with dicobalt octacarbonyl. Oxidative additions of 1-iodoperfluoroalkanes on the cobalt(I) complexes provided cobalt(III) complexes with one of their four ponytails bonded directly to the metal and with a stereocenter at the metal. [Ref. 16]

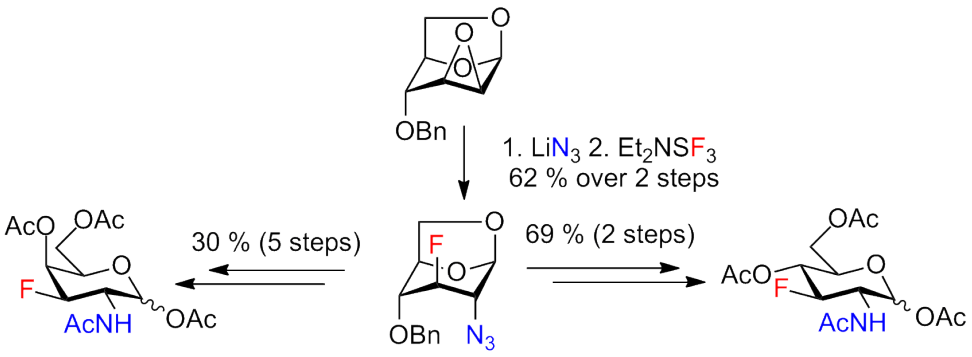


Synthesis of cobalt(I) dicarbonyl complexes and oxidative addition of iodo(perfluoro)alkanes

A convenient route to peracetylated 3-deoxy-3-fluoro analogs of D-glucosamine and D-galactosamine from a Černý epoxide

(J. Karban, karban@icpf.cas.cz; supported by ICPF)

1,6:2,3-dianhydro-4-*O*-benzyl-β-D-mannopyranose has been conveniently transformed into peracetylated 3-deoxy-3-fluoroanalogues of D-glucosamine and D-galactosamine in four or six steps, respectively, in an overall yield of 43 % or 19 %, respectively. In addition, our approach furnished selectively protected fluorohydrins which are useful synthetic intermediates with potential for a regioselective functionalization or glycosylation at C4. Investigation towards this application and an extension of our methodology to other fluorinated hexosamines is currently underway in our laboratory. [Ref. 9]

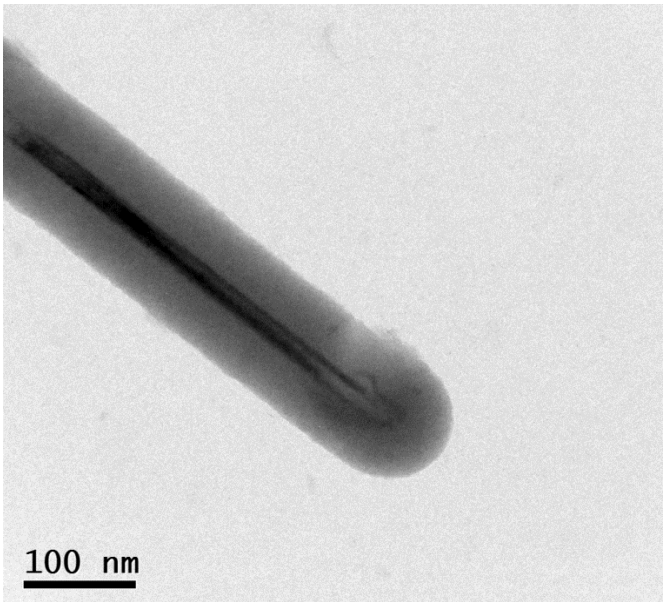


Peracetylated 3-deoxy-3-fluoro analogs of d-glucosamine and d-galactosamine

Silicon Nanowires Grown on Metal Substrates via Self-Catalyst Mechanism

(V. Dřínek, drinek@icpf.cas.cz; supported by GACR, project No. 13-25747S)

Low Pressure Chemical Vapor Deposition (LPCVD) was applied to grow Silicon Nanowires (SiNWs) without any heteroatom catalyst or special pretreatment of substrates used. Silane (SiH_4) as a precursor was pyrolyzed at 500 °C in an oven at molybdenum or iron substrates. NWs were several microns long, about 100 nm thick and possessed core-jacket structure. The thin core is composed of crystalline silicon oriented in <110> direction whereas the jacket is amorphous silicon. Unlike other approaches this one makes possible to avoid contamination caused by metal heteroatom seeds and/or applying special procedures for substrate pretreatment initializing/supporting NW growth. [Ref. 5]



A silicon nanowire with distinguished crystalline core and amorphous jacket

Novel sensors based on laser ablated graphene

(R. Fajgar, fajgar@icpf.cas.cz; supported by NATO, project No. 984399)

Graphene layers deposited by excimer laser ablation technique on a glass substrate were covered with silver and silver/gold alloy nanoparticles. The ability for Surface-Enhanced Raman Scattering (SERS) was demonstrated. In vacuum, metal nanoparticles with diameter between 10 and 25 nm reaching the polymer/graphene substrates induce graphitization of the graphene sheets as revealed by Raman spectroscopy. Ablation conditions were optimized to preserve graphene layers as a substrate for metal nanoparticles deposition in helium and argon atmosphere. The nanocomposites were characterized by means of spectroscopy, microscopy and diffraction techniques. The SERS substrate performance was tested using model compounds. Highly enhanced signal was observed and sensoric properties of the novel substrates were demonstrated. The substrates were optimized for detection of compounds, interesting from technological and medical aspects (e.g. methylviolet B, arsenazo, beryllon). [Ref. 15]

Sensoric properties of reduced graphene oxide/polymer composite towards pressure changes were demonstrated. The -OH functionalities on the rGO platelets and in the polymer chains were used as reactive sites, linked by the presence of NCO terminated polyurethane prepolymer. The film possesses improved mechanical properties and good bulk electrical conductivity, highly dependent on pressure changes. A sensor study was performed using a

developed device allowing to vary the impacting pressure continually. The mechanical pressure was changed and corresponding resistivity was recorded. The resistance was decreasing by 50% in a range from 0 to 0.2 MPa. Especially low pressures have important influence on the resistivity of the samples. We expect that mechanical pressure influences distribution of the graphene nanoplatelets in the composite which results in resistance changes. [Ref. 2]

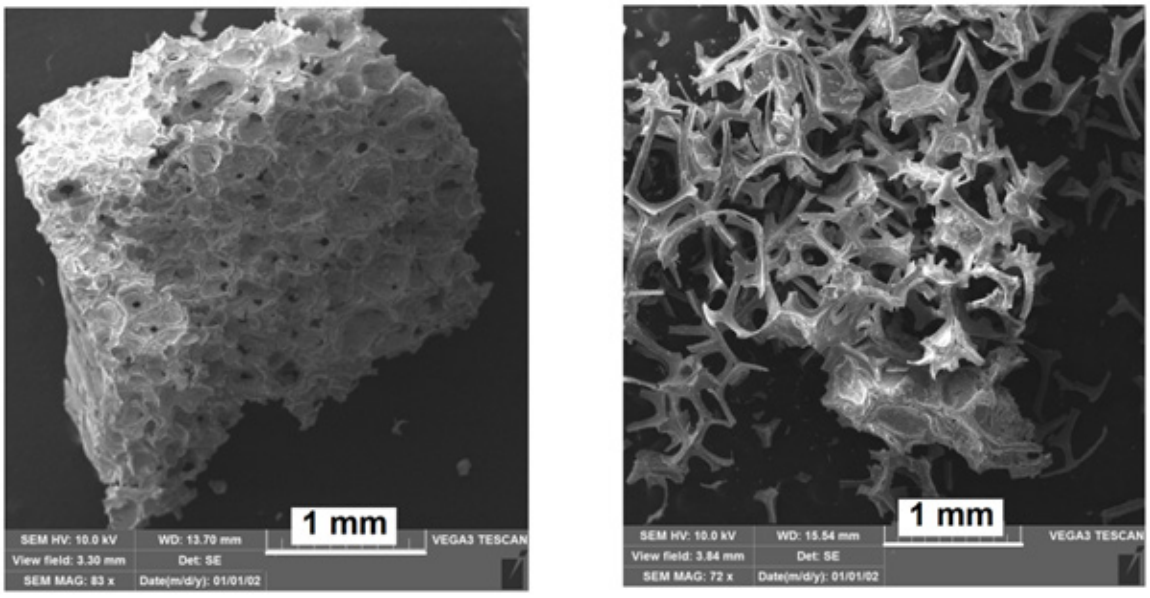
Highly efficient catalyst and process for degradation of resistent antibiotics

(J. Pola, pola@icpf.cas.cz; supported by TACR, project No. TA04020860)

The aim of the project is (a) the development and efficiency verification of a new-type nanocomposite heterogeneous catalysts for technological process of advanced oxidative degradation of refractory antibiotics occurring in waste waters, (b) the development and optimization of a model reactor for this process, (c) the development and optimization of a model technological process in combination with MBBR system for biological waste water post-treatment. The novel catalysts based on grains of ferrous spinels will be laser-immobilized on high surface mesostructured walls of macroporous glass/ceramic carriers and will have high priorities in efficient adsorption of pollutant molecules to high-surface mesoporous glass structure and in pollutants degradation taking place exclusively on the incorporated grains.

The catalytic systems will be prepared by laser ablative deposition from the bulk precursors using different laser irradiation sources, they will be characterized by physical and spectral methods before and after hydroperoxide treatment, and their catalytic efficiency in decomposition of hydroperoxide and degradation of a model refractory pollutant will be evaluated and compared.

Successful solution of partial objectives will significantly improve current complex technology for waste water treatment by additional decontamination stage. The suggested technology will prevent escape of resistant antibiotics and will decrease the content of residual products of waste water biological treatment to surface waters and will thereby eliminate increasing harmful effects of these drugs and other organic compounds in ecosystem.

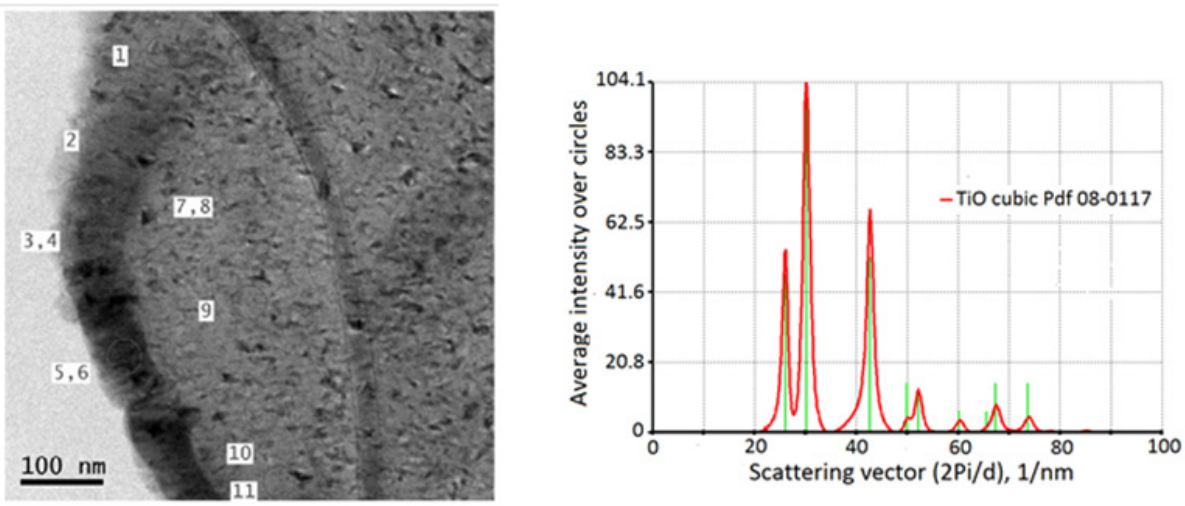


Representative structures of sol-gel-prepared samples of porous glass

Porous and macroporous titanium surfaces with embedded submicrometer-sized Si-, SiO_x- and TiO_x- moieties for enhancing bone osseointegration and adhesion to titanium implants

(J. Pola, pola@icpf.cas.cz; supported by TACR, project No. TA04010169)

The main goals of the project are the development and optimization of a new-type of biocompatible surfaces of titanium implants for enhanced osseointegration and adhesion of bone tissue, a know-how for the production of the novel model implants, and finally the fabrication of model samples for commercial sphere. The partial goals are (a) fabrication of macroporous surface layers of bulk titanium by using laser radiation-induced structural modification of titanium, (b) penetration of sol-gel polymerizing titania and silica precursors into these layers to achieve macro-porous bicontinuous titanosilicate structures, (c) laser-induced incorporation of SiO_x and TiO_x nanoparticles and hydrated SiO_x and TiO_x nanoparticles into these structures catalyzing the growth of bone tissue, and (d) incorporation of hydroxyapatite grains into these structures, which will serve as seeds of growing bone tissue.



TEM and EDS of films deposited by ArF laser ablation of titanium monoxide

International co-operations

Centre for Environmental Biotechnology, University of Tennessee, Knoxville, TN, USA: Improved biomaterials for the encapsulation of living cells

Environmental Sciences Division Oak Ridge National Laboratories, Oak Ridge, TN, USA: Application of nanomaterials and novel organic-inorganic materials in optical sensors

Graz University of Technology, Graz, Austria: ^{29}Si and ^{119}Sn NMR

Institut de Chimie Moléculaire de Reims, CNRS 7312, France: ESI-MS of titanocene-containing dendrimers

Lehrstuhl für Organische Chemie I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany: Chemistry of hetero[*n*]phenacenes

Faculty of Technology and Metallurgy, University of St. Cyril & Methodius, Skopje, Republic of Macedonia: Preparation of SERS active substrates based on graphene

King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia: Preparation of Ag/C nanocomposites by laser-induced carbonization of n-hexane

Southeast University, Department of Physics, Nanjing, China: Preparation of Ag/C nanocomposite by laser–induced carbonization of n-hexane

POLYMAT, Institute for Polymer Materials, San Sebastian, Spain: Laser ablation of graphene-based composites

Visitors

Despina Spaseska, University of St. Cyril & Methodius, Skopje, R. Macedonia
Akihiko Ouchi, National Institute of Advanced Industrial Research and Technology, Tsukuba, Japan
Helena Grennberg, Uppsala University, Sweden

Teaching

J. Čermák: UJEP, Faculty of Science, courses "Organic Chemistry I and II", "Chemistry of Heterocyclic and Organometallic Compounds", "Introduction to the Spectral Methods in Organic Chemistry"
G. Kuncová: UCT, Faculty of Chemical Engineering, postgraduate course "Optical Sensors for Measurement in Chemical and Biological Reactors"

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Original papers

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[10] Lísal M., Chval Z., Storch J., Izák P.: Towards Molecular Dynamics Simulations of Chiral Room-Temperature Ionic Liquids. *J. Mol. Liq.* 189(SI), 85-94 (2014).

[11] Lyutakov O., Hejna O., Solovyev A., Kalachyova Y., Švorčík V.: Polymethylmethacrylate Doped with Porphyrin and Silver Nanoparticles as Lightactivated Antimicrobial Material. *RSC Adv.* 4(92), 50624-50630 (2014).

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[16] Strašák T., Čermák J., Červenková Šťastná L., Sýkora J., Fajgar R.: Cobalt(I) and Cobalt(III) Cyclopenta-dienyl Complexes with New Silicon-branched Fluorous Tags. *J. Fluorine Chem.* 159, 15-20 (2014).

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Fields of research

- Environmental organic chemistry and microwave photochemistry
- Advanced processes for Waste-to-Energy (WtE)
- Cleaning of syngas from fluidized-bed gasification of coal-biomass blends
- Advanced processes for gasification, gas cleaning and hydrogen production
- Persistent organic pollutants and heavy metals emissions and behaviour
- Urban mining - metals recovery from waste ashes

Applied research

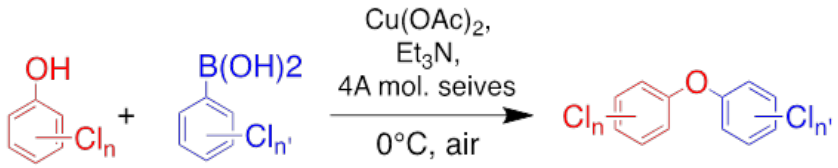
- Brownfields - Source of renewable energy
- Development of a pilot plant for monitoring of Hg emissions reduction
- Design optimization of multi-stage biomass gasifier generating gas with low tar content
- Co-combustion of coal and rubber granulate in a fluidized bed
- New gas refining technology for small and mobile thermal waste degradation units
- Wet precipitators PM for medium-power boilers burning renewable biomass
- Production of paper products with special properties from waste security paper
- In-situ thermal desorption with applications of microwaves
- Development and verification of thermal desorption technology using microwaves
- Advanced method using microwaves for repair of damaged roads
- Progressive method and new equipment using microwaves for drying of surfactants
- Revolutionary method using microwaves for the chemical depolymerization of waste polyethylene terephthalate (PET)

Research projects

Applications on the field of environmental organic chemistry and microwave photochemistry

(V. Církva, cirkva@icpf.cas.cz; supported by ICPF; TACR, project No. TA01010646)

An efficient synthesis of polychlorinated diphenyl ethers (PCDEs) using the $Cu(OAc)_2$-catalyzed Chan-Lam coupling reaction has been described. A library of all possible mono- and dichlorinated diphenyl ether congeners was prepared and characterized using MS, ^1H, and ^{13}C NMR spectroscopy, and Kovats retention indices. Our approach, using the optimized reaction conditions (i.e., reaction temperature, oxidizing atmosphere and base), significantly improves and simplifies the process compared to previously reported syntheses [Ref. 1].



Copper mediated synthesis of mono- and dichlorinated diaryl ethers

The coupled activation of photochemical reactions by using of two different types of radiation, microwave and UV/Vis, is covered by the new discipline called microwave photochemistry. Such a connection might have a synergic effect on reaction efficiencies or, at least, enhance them by summing up the individual effects. The objective of this discipline is frequently, but not necessarily, connected to the electrodeless discharge lamp (EDL) as a novel light source which generates efficiently UV/Vis radiation when placed into a microwave field. We have applied this concept on photochemical synthesis of helicenes and phenacenes [Ref. 6].

Experimental set-up for microwave photochemical experiments with EDLs

Waste-to-Energy Competence Center

(M. Šyc, syc@icpf.cas.cz; joint project with Brno University of Technology, EVECO Brno s.r.o., ZVVZ-Enven Engineering a.s., PBS INDUSTRY a.s., ČEZ a.s., supported by TACR, project No. TE02000236)

Waste-to-Energy (WtE) Competence Centre activities are aimed at increasing competitiveness of the Czech Republic in the field of WtE. Activities are specified in such a way to be able to cover WtE from a primary idea to final products based on recent results of strategic planning, selection and design of up-to-date technologies and equipment. One of the main aims of the consortium is the development of small scale waste-to-energy plant (with capacity below 40 kt/year).

ICPF is leader of work package focused on innovation and re-design of components of WtE with respect to overall energy optimization and increase of efficiency.

Our research interests/tasks can be summarized as follows:

- Optimization of dry cleaning methods with simultaneous flue gas deNO_x and dioxin removal on catalytic bag filters, handling of spent sorbents, etc.;
- MSWI solid residuals (bottom ash and fly ashes) utilization and development of methods for recovery of non-ferrous metals, precious metals, REE etc. and application of selected fraction in construction industry;
- Sewage sludge combustion and co-combustion with other waste fuels;
- Phosphorus recovery from sewage sludge ash.

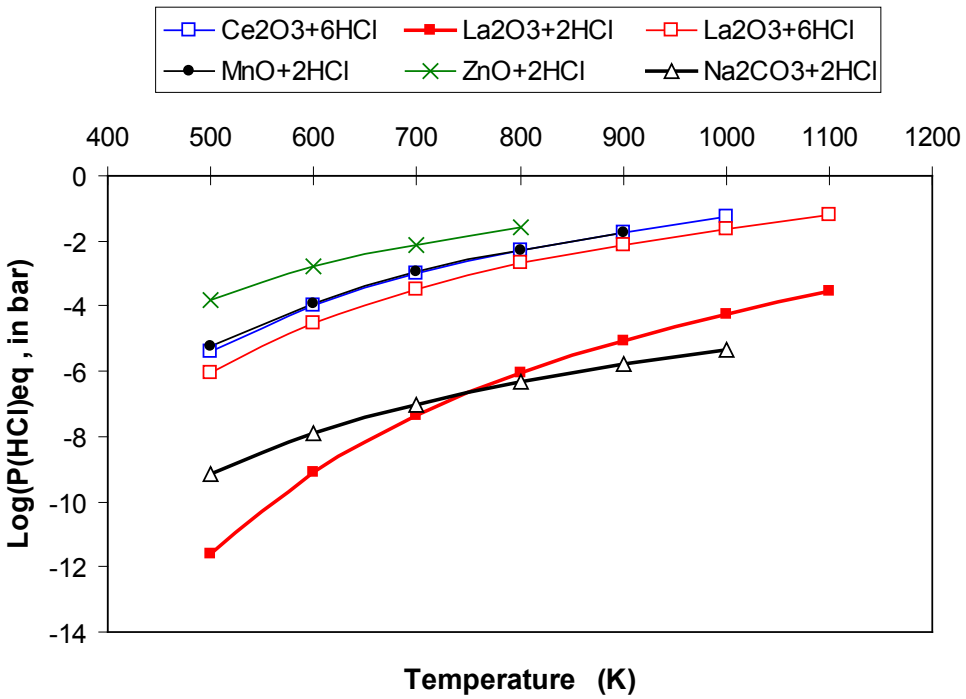
Valuable components in MSWI bottom ash

Cleaning of syngas from from fluidized-bed gasification of coal-biomass blends for advanced power generation

(K. Svoboda, svoboda@icpf.cas.cz; bilateral research project (NSC Taiwan) with INER - Taiwan; supported by GACR, project No. 14-09692J, reg. number of the foreign project: 102WBS0300011)

The research is aimed at study and solution of problems (thermodynamic constraints, reactivity, capacity and deactivation of the sorbents, textural changes, interferences of HCl) in

removal of sulfur compounds from fuel gas by solid sorbents at temperatures 400-600 °C. A soda-based sorbent are used for pre-cleaning of syngas and for study of important effects of accompanying gases (mainly, H_2S, naphthalene) and temperature on the sorption process of HCl. Sorbents based on ZnO and CeO_x serve for removal of H_2S, COS, destruction/removal of thiophene and for study of the intereferences (CO_2, H_2O(g), HCl, naphthalene). For characterization of sorbents, TG, XRD, SEM/EDS, textural and other tools are employed. The sorption reactions are studied by means of a differential, fixed-bed reactor and by an integral fluidized-bed reactor. Theoretical models with simplified reaction kinetics and particle structure for description and analyses of sorption process in fixed and fluidized bed will be developed and solved. [Refs. 5, 7, 9, 18]

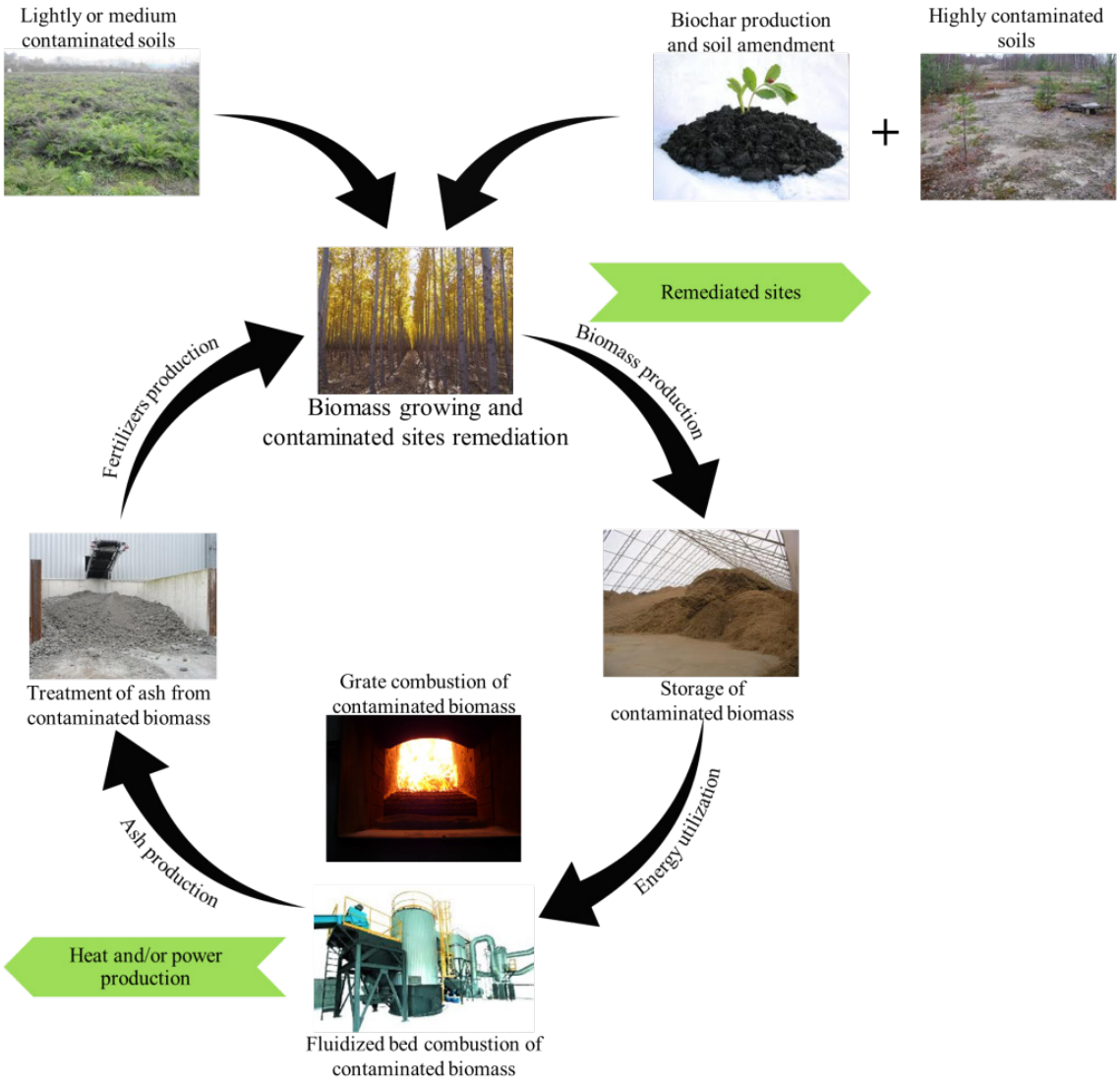


Dependence of equilibrium HCl pressures on temperature for ZnO, MnO, La_2O_3 and Ce_2O_3 solid sorbents (assumed P_{H2O} = 0.1 bar, P_{CO2} = 0.2 bar) - comparison with equilibrium HCl pressure in the reaction of HCl with soda

Brownfields - source of renewable energy

(M. Šyc, syc@icpf.cas.cz; joint project with EVECO Brno s.r.o. and CULS; supported by TACR, project No. 01020366)

The phytoextraction ability of some fast-growing plant species leads to the idea of connecting biomass production with soil remediation on contaminated industrial zones and regions. This biomass will contain significant amount of heavy metals and its energetic utilization has to be considered carefully to minimize negative environmental impacts. Therefore, the behavior of selected heavy metals was observed during thermal treatment of contaminated biomass. Moreover, a detailed analysis of trace and nutrient elements distribution and chemical speciation in ashes was performed. The potential of the application of these ashes and methods of treatment for heavy metals removal was evaluated. This knowledge is essential for further utilization of all products of gasification and for the fulfillment of emission limits during combustion. The concept of contaminated biomass growing and utilization was proposed. [Refs. 11, 21, 22]



The concept of contaminated biomass growing and utilization

Development of a pilot plant for monitoring of Hg emissions reduction from large and medium capacity energy sources

(V. Veselý, vesely@icpf.cas.cz; joint project with ÚJV Řež a.s., ENVIRMINE-ENERGO, a.s. and Technical University Ostrava; supported by TACR, project No. TA04020723)

The objective of the project is identification of the issue concerning meeting of presumed Hg emission limits in single energy sources burning fossil fuels in the Czech Republic and a draft of technical and economical solution to meet predicted Hg emission limits at fossil fuel burning. Measurement in the existing energy sources will be performed to determine concentration of Hg in flue gas in forms of Hg^0 (gaseous atomic mercury), Hg^{2+} (oxidized mercury) and Hg^P (gaseous Hg bonded with solid particles, such as fly ash and combustible carbon in the fly ash).

The effects of operating conditions and selective catalytic reduction on Hg concentration in flue gas will be investigated on a developed pilot plant. The result of the project solution will serve as basis for technical documentation for the existing energy sources modifications, or preliminary documentation of new plants determined for Hg emission elimination.

Design optimization of multi-stage biomass gasifier generating gas with very low tar content

(M. Pohořelý, pohorely@icpf.cas.cz; joint project with TARPO spol. s r.o. and University of Chemistry and Technology, Prague; supported by TACR, project No. TA04020583)

The aim of this project is full utilization of the main advantages of a multi-stage gasification concept using the original know-how of the unique multistage gasifier Tarpo. The goals of the project are to increase the efficiency of cold gas efficiency (from the raw fuel) to a value of min. 89%, which can increase the efficiency of power generation in the combustion engine to a value of 32% and for modern engines to an efficiency of 36%. On the basis of the above equipment three thermal power stations are operated in the Czech Republic and additional three are under construction (2 in Czech Republic, 1 in Slovakia). [Refs. 8, 9]

Combined heat and power generation plant in Kozumín – under construction

Co-combustion of coal and rubber granulate in a fluidized bed

(M. Pohořelý, pohorely@icpf.cas.cz; joint project with PATREM PIPE TECHNOLOGIES, s.r.o. and Alpiq Generation (CZ), s.r.o.)

It has been demonstrated how to effectively co-combust commonly used brown and black coal with rubber granules in fuel blends containing up to 15 wt. % of rubber granules. Combustion investigations have been carried out in our experimental fluidized-bed reactor as well as in a commercial heating plant in Zlín with the circulating fluidized-bed boiler K31 (Alpiq Generation s.r.o.).

Fluidized bed reactor at ICPF

New gas refining technology for small and mobile thermal waste degradation units

(V. Veselý, vesely@icpf.cas.cz; joint project with SMS CZ, s.r.o. and ALG Europe, s.r.o.; supported by TACR, project No. TA03020880)

Within project scope was developed a compact technology for high efficiency dry refining flue gas technology for small and mobile incinerators. This refining technology is consisted of three separate stages of cleaning, which are arranged in a logical sequence and serves to maximize the refining effect. The primary stage of treatment is based on the use of crushed limestone as the raw high-temperature catalyst, the secondary stage is purifying flue gas from acidic and heavy metals components in the flue gas by sprayed milled waste from the primary stage of treatment and tertiary treatment are stationary filter, which consists of a new type of sorbent-based product Chezacarb, which is produced as a waste product of hydrogen production from partial oxidation in Unipetrol RPA. These cleaning elements under specified conditions of temperature and residence time are able to remove tar residues from the flue gases, VOCs, acid gases and especially PCDD/F and PCB and mercury vapor without wet scrubber at any stage of cleaning. This allows you to use this system in the areas where is no sustainable water management options.

Research and development of wet precipitators PM for medium-power boilers burning renewable biomass

(J. Hanika, V. Veselý, hanika@icpf.cas.cz, vesely@icpf.cas.cz; joint project with TENZA, a.s., Brno and VSB-TU Ostrava; supported by TACR, project No. TA02020369)

Project is developed the new technology for separating solid particles from flowing mass of air, especially for middle-burning source of renewable biomass resources and the technology present in the form of a utility model and a prototype of representative size. The

size of the prototype was chosen to allow transfer of results of experimental research and development in commercial use after project completion.

Wet separator for flying ash

Production of new kinds of paper products with special properties from waste security paper

(J. Sobek, sobek@icpf.cas.cz; joint project with SPM - Security Paper Mill, a.s.; supported by TACR, project No. TA04010051)

Project is aimed at creating new product portfolio derived from paper with new antimicrobial and thermal insulation properties. The technology will utilize waste security paper. Due to falsification concerns discarded material is used for energetic purposes only so far (i.e. is burnt). The sub-objective is the development of unique antibacterial fillers and insulating fillers exploiting PET waste materials. The technology will led to reduction of natural resources usage and is environmentally friendly owing to exploitation of recycled component materials (security paper and PET). Newly developed products with added value are designated for immediate commercialization and market entry. High quality security paper with new properties produced by Neograph a.s. will further increase competitiveness of the principal beneficiary.

In-situ thermal desorption with applications of microwaves

(J. Sobek, sobek@icpf.cas.cz; joint project with Dekonta a.s.; supported by TACR, project No. TA04020981)

The aim of the project is to develop and verify a method of an in-situ thermal desorption with use of microwaves. One of the results would be a technical-economical study which would be based on results obtained from pilot tests of new microwave technology and also from comparison of other methods of in-situ thermal desorption as electrical heating, steam enhanced extraction or gas heating. Of course, part of the output would be the patent and

utility models of new technology and constructed technical parts as waveguides. To present the results of the project is also one of the project's aims. If other companies and specialists who deal with environment protection know about the new technology and it's benefits, the expected gains will be reached. [Ref. 19]

Development and verification of thermal desorption technology using microwave radiation

(M. Hájek, J. Sobek, hajek@icpf.cas.cz, sobek@icpf.cas.cz; joint project with UCT and Dekonta, a.s; supported by TACR, project No. TA01020383)

The main goal of the project was the development and verification of thermal treatment method utilizing microwave radiation for heating up contaminated material in a primary treatment unit. An originally designed pilot-scale treatment unit was assembled. Operation efficiency of the unit was verified by treatment of wide range of contaminated soil and solid waste samples. By development of this innovative technology, the applicant is able to strengthen his market position and improve his competitiveness on the field of remediation services and hazardous waste treatment activities.

In this study, were compared efficiencies of persistent organic pollutants (POPs) removal from solid materials (soil and building waste) using conventional and microwave heating. These experiments were performed in laboratory apparatus and pilot scale devices. It was confirmed that more polar pollutants (for example chlorinated pesticides) can be effectively removed at a temperature below their boiling point. Probably, this effect was evoked through co-transport some contaminants with water vapour. Microwave heating was a very applicable alternative heating method that brings about faster heating of the material and saving of energy. The examined groups of pollutants (pesticides and PCBs,) were removed with high efficiency at temperatures around 250 °C. [Refs. 14, 15, 16, 19]

Pilot equipment for microwave thermal desorption (Dekonta a.s.)

Advanced method using microwaves for repair of damaged roads

(M. Hájek, J. Sobek, hajek@icpf.cas.cz, sobek@icpf.cas.cz; supported by FUTTEC a.s.)

New and modern method of microwave heating was applied for repairing roads with asphalt material. The aim is year-round repair of the local surface cracks, joints or pot holes which have arisen during winter season.

The quality tests of repaired place showed that after 3 years good quality of repaired place by microwave heating was obtained. Present research is now focused on reparation of roads with low absorption for microwaves. [Ref. 12]

Progressive method and new equipment using microwaves for drying of surfactants

(M. Hájek, J. Sobek, hajek@icpf.cas.cz, sobek@icpf.cas.cz; supported by CHEMPHARM Engineering, s.r.o.)

The method and equipment making use of microwaves was applied on drying of surfactants from water solutions. It was found that use of microwave heating provides better quality of dried surfactants compared to conventional method. Drying was performed under mild condition and was found that process was significantly energy saving. The aim was to prepare such different surfactants (anion-active, cation-active, non-ionic, and/or amphoteric) in powder form having a high quality. [Refs. 13, 20]

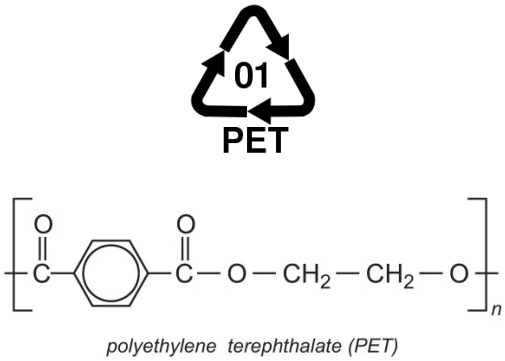
Microwave reactor

Revolutionary method using microwaves for the chemical depolymerization of waste polyethylene terephthalate (PET)

(M. Hájek, J. Sobek, hajek@icpf.cas.cz, sobek@icpf.cas.cz; supported by NOEN, s.r.o.)

New technology has been developed in order to solve problems of growing production and accumulation of waste PET bottles. This recycling technology is based on use of microwave energy for PET depolymerization and it is characterized by low energy consumption and by high purity of products (terephthalic acid, monoethylene glycol) so called "Polymer Grade" quality. It was tested on pilot plant with capacity 1-10 kg/h PET bottles with MW reactor of 0.12-1.0 m^3.

One advantage of this method over others is that it does not require sorting before processing. This new technology is protected by patent documents both in the Czech Republic (CZ299908) and in 5 countries (EP2176327), in Germany, Italy, France, UK and in China. Recently the technology was sold to the Polish company NRT Polska Sp. Z.o.o. Successful technology was verified on microwave reactor with working capacity of 280-1000 L. In 2013 was started in Poland the construction of factory with capacity of 10 000 ton of PET per year. [Refs. 2, 3, 4, 17, 23]



Recycling technology based on use of microwave energy for PET depolymerization

International co-operations

Central Mechanical Engineering Research Institute, Durgapur, India: Waste gasification
Institute for Energy and Transport, Joint Research Centre of EC, Petten, the Netherlands: Atmospheric and pressurized fluidized bed combustion/gasification technologies; Waste incineration/gasification
University of KwaZulu-Natal, Durban, Republic of South Africa: Gaseous and particulate emissions
The Vienna University of Technology, Austria: Fluidized bed biomass gasification
Imperial College, London, United Kingdom: Pressurized FB gasification, combination with SOFC
The Combustion Research Institute, National Research Council, Napoli, Italy: In-bed catalytical processes for fluidized bed gasification and tar reduction
Institute of Nuclear Energy Research, Atomic Energy Council, Taiwan: Development of fluidized bed gasification with efficient gas cleaning, chemical looping production of hydrogen
Laboratório Nacional de Energia e Geologia, Portugal: Syngas cleaning, removal of tar, sulfur and nitrogen compounds

Visitors

M. Čárský, University of Kwazulu-Natal, Durban, Republic of South Africa
Y.-P. Chyou, Institute of Nuclear Energy Research (INER), Taiwan

Teaching

V. Církva: UCT, Faculty of Chemical Technology, postgraduate course "Microwave Chemistry"
V. Církva: UCT, Faculty of Chemical Technology, postgraduate course "Photochemistry"
M. Pohořelý: UCT, Faculty of Environmental Technology, postgraduate course "Energetic Using of Biomass" and courses "Alternative Energy Sources I", "Chemical Calculations", "Laboratory of Fuel Analysis", and "Laboratory of Fuels"
M. Punčochář: Czech University of Life Sciences Prague, course "Renewable and Alternative Sources of Energy"
K. Svoboda: UJEP, Faculty of Environment, courses "Decontamination and Bio-remediation Technologies" and "Energetics (Power generation) and Protection of the Environment"

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Competence centre for biorefining research (BIORAF)

BIORAF project (TE01020080), supported by the TACR, employs the techniques of green chemistry for biomass utilization to the high added-value products and energy sources. By refining, it is possible to obtain food supplements, fodders and fertilizers, new-generation biofuels and energy from the biomass of microbial, plant or animal origin. Biorefining is a unique way of new sustainable substitution of fossil fuels minimizing the adverse effect on environment while exploiting the whole volume of biomass.

Joint organizations:

- Institute of Chemical Process Fundamentals
- Institute of Chemical Technology, Prague
- Institute of Botany of the CAS
- Rabbit Trhový Štěpánov, a.s.
- Agra Group, a.s.
- Briklis, spol. s r.o.
- EcoFuel Laboratories, spol. s r.o.

BIORAF
Centrum kompetence pro výzkum biorafinací

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Scientific director of the Centre: Ing. Olga Šolcová, CSc., DSc.

Technological director of the Centre: Prof. Ing. Jiří Hanika, DrSc.

Project web pages (http://bioraf.icpf.cas.cz/) provide up-to-date information about projects results, milestones and events.

Biorefinery research centre of competence

(O. Šolcová, solcova@icpf.cas.cz)

In a relatively short period of time, the project established interdisciplinary research centre which resulted in applications in livestock breeding, cultivation and plant protection, food supplements and health care. The companies involved in the project not only supply so far unused waste materials, but already implement and benefit from the project results; new design of bioreactors and knowledge on algae cultivation find use in novel poultry feeding, plant extracts and waxes are tested for cosmetics production and as a repellent for protection of forests, new species of microalgae extremely rich in omega-3 fatty acids are being licensed for production of pharmaceuticals and food supplements, new process equipment are manufactured etc.

Selection of unicellular algae strains capable of growth on the raw glycerol belongs to the project results as well cultivation of microorganisms for the production of biomass rich in Docosahexaenoic acid applicable as food additives, photobioreactor for cultivation of microalgae, and the novel verified technology Inulin from the tuber of Jerusalem artichoke - certification of crop cultivation in which framework the agent for plant protection against insects was developed. In the framework of processing technology of waste feathers the pressure hydrolysis of chicken cartilage and feathers protein wastes, which is focused on the production of valuable amino acids mixtures with nutraceutical importance, was developed. Moreover, variety of prototypes suitable for mixing, disintegration, drying, pelleting,

briquetting, packing, storage or transport were developed as the side products and some of them were also produce for sale. Majority of products is focused on private customers from the Czech Republic and also abroad. In the first part of the Project majority of technologies was suggested and developed on laboratory level and only some technologies and products were scaled up. Nowadays, a scale up of all products and technologies is planned

Project brought awareness into society about the biorefinery area as new scientific direction, that in Czech Republic was virtually absent before creation of BIORAF, but has big perspective for development of small and medium size companies. BIORAF published through Academia publishing house a free book on this subject to educate public and scientific community.

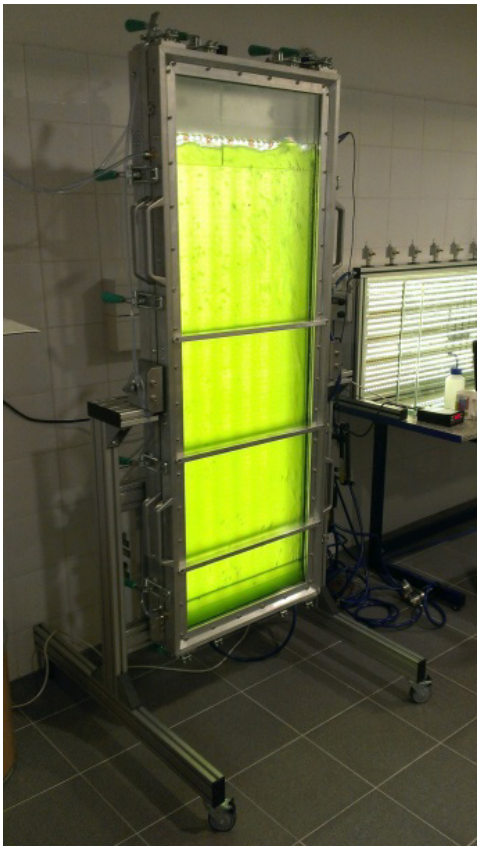

Photo-bio-reactor

Feathers as reusable materials

Method for processing algae and cyanobacteria

(J. Sobek, V. Veselý, sobek@icpf.cas.cz, vesely@icpf.cas.cz)

The method for processing algae and blue-green algae to obtain oil by breakage of their cell wall with the use of microwave radiation has been applied. Water suspension of algae was first adjusted by the addition of a hydrophobic sorbent in an amount ranging from 0.5 to 5 % by weight and so adjusted suspension was heated at a pressure in the range of about 200 to about 2000 kPa by the action of microwave radiation to a temperature in the range of 105 to 190 °C for a period of 1 to 5 minutes. Subsequently, the suspension was led to expand and after cooling down and separation of disintegrated algae, the sorbent with sorbed oil was separated from the water layer wherein the sorbed oil was then isolated by extracting agent. [Ref. 1]

Sedimentation of algae

Method and device for hydrolysis of inulin solution

(J. Sobek, V. Veselý, sobek@icpf.cas.cz, vesely@icpf.cas.cz)

Inulin represents a mixture of polysaccharide molecules with the general formula GF_{n-1}, where G is glucose, F is fructosyl, and *n* is degree of polymerization (polycondensation). It was obtained from Jerusalem artichoke from underground part.

Method of hydrolysis of inulin from natural juice was based on membrane electrodialysis device, in which the anode compartment was fed a solution of natural juices containing inulin. This solution was treated together with mineral salts from a previous separation of juice. In the cathode compartment provided a hydrolyzate formed in the anode compartment. [Ref. 2]

Root of topinambour and process of drying

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[1] Sobek J., Hájek M., Veselý V., Punčochář M., Církva V.: Způsob zpracování řas a sinic. The Processing of Algae for Obtaining Oil Resulting. *Pat. No. 304392*/PV 2013-323. Applied: 13.04.30, Patented: 14.02.26.

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J. HANIKA: "Hemijska Industrija/Chemical Industry"
J. HANIKA: "Pharmaceutical Design and Current Perspectives"
P. IZÁK: "Chemical Papers"
K. JEŘÁBEK: "Reactive and Functional Polymers"
P. KLUSOŇ: "ChemBioEng Reviews"
J. KŘIŠŤÁL: "Chemical Engineering & Technology" (guest editor of special CHISA issue)
G. KUNCOVÁ: "International Journal of Sensors and Sensor Networks"
I. NEZBEDA: "International Journal of Liquid State Sciences"
I. NEZBEDA: "Journal of Atomic and Molecular Physics"
I. NEZBEDA: "Molecular Physics"
M. PUNČOCHÁŘ: "Scientific Papers of the University of Pardubice, A"
J. SMOLÍK: "Aerosol and Air Quality Research"
J. SMOLÍK: "Heritage Science"
J. SÝKORA: "Journal of Crystallography"
I. WICHTERLE: "Kemija u Industriji"

Memberships in International Bodies

K. AIM: Senior Vice Chairperson, Board of Governors, Joint Research Centre, European Commission (http://ec.europa.eu/dgs/jrc/index.cfm?id=5500)
K. AIM: Working Party on Thermodynamic and Transport Properties, European Federation of Chemical Engineering (http://www.wp-ttp.dk/index.php/people)
K. AIM: Member, Permanent International Steering Committee of European Symposia on Applied Thermodynamics (http://www.esat2014.org/steering.html)
M. BENDOVÁ: Working Party on Fluid Separations, European Federation of Chemical Engineering (http://www.efce.info/Members-p-111943.html)
M. BENDOVÁ: IUPAC Analytical Chemistry Division, Subcommittee on Solubility and Equilibrium Data (http://www.iupac.org/home/about/members-and-committees/db/division-committee.html?tx_wfqbe_pi1[publicid]=502)
M. BENDOVÁ: Management Committee Member, EU COST Action CM1206 EXchange on Ionic Liquids (EXIL) (http://www.cost.eu/COST_Actions/cmst/Actions/CM1206)
G. BOGDANIĆ: Working Party on Thermodynamics and Transport Properties, European Federation of Chemical Engineering (http://www.wp-ttp.dk/index.php/people)
J. ČERMÁK: Chair, European Association for Chemical and Molecular Sciences - Division of Organometallic Chemistry (http://www.euchems.eu/divisions/organometallic-chemistry.html)
J. DRAHOŠ, Executive Board Member, Working Party on Multiphase Fluid Flow, European Federation of Chemical Engineering (http://www.multiphase-efce.org/members.php)
J. HANIKA: Working Party on Chemical Reaction Engineering, European Federation of Chemical Engineering (http://www.efce.info/Members-p-109427.html)
P. IZÁK: Elected Vice-President of the „European Membrane Society Board"
M. RŮŽIČKA: Executive Board Member, Working Party on Multiphase Fluid Flow, European Federation of Chemical Engineering (http://www.multiphase-efce.org/members.php)
M. RŮŽIČKA: Member of European Multiphase Sciences Institute (EMSI), Coordinator for Chemical Reactor Systems
J. SMOLÍK: Member of the Council of the European Aerosol Assembly (EAA) (http://www.gaef.de/eaa/)
H. SOVOVÁ: Working Party on High Pressure Technology, European Federation of Chemical Engineering (http://www.efce.info/Members-p-717.html)
J. STORCH: Management Committee Member, EU COST Action MP1406 Multiscale in Modelling and Validation for Solar Photovoltaics (MultiscaleSolar) (http://www.cost.eu/COST_Actions/mpns/Actions/MP1406)
V. ŽDÍMAL: Member of the Council of the European Aerosol Assembly (EAA) (http://www.gaef.de/eaa/)
V. ŽDÍMAL: Management Committee Member, EU COST Action MP1404 Simulation and pharmaceutical technologies for advanced patient-tailored Inhaled medicines (SimInhale) (http://www.cost.eu/COST_Actions/mpns/Actions/MP1404)

16TH E. HÁLA LECTURE (2014)

ANDREAS SEIDEL-MORGENSTERN (Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany), on 10 November 2014:
"Process to separate enantiomers"

ACRONYMS USED THROUGHOUT THE REPORT

ASCR	Academy of Sciences of the Czech Republic
BAS	Bulgarian Academy of Sciences
CAS	Czech Academy of Sciences
CFD	Computational Fluid Dynamics
CNRS	Centre Nationale de la Recherche Scientifique
CTU	Czech Technical University in Prague
CU	Charles University in Prague
CULS	Czech University of Life Sciences Prague
CVD	Chemical Vapor Deposition
EC	European Commission
EFCE	European Federation of Chemical Engineering
EU	European Union
FP	Framework Programme
GACR	Grant Agency of the Czech Republic
HDS	Hydrodesulfurization
IBOT	Institute of Botany of CAS, v. v. i., Průhonice
ICPF	Institute of Chemical Process Fundamentals of the CAS, v. v. i., Prague
IIC	Institute of Inorganic Chemistry of the CAS, v. v. i., Prague
IL	Ionic Liquid
IMC	Institute of Macromolecular Chemistry of the CAS, v. v. i., Prague
IR	Infrared
JH IPC	J. Heyrovský Institute of Physical Chemistry of the CAS, v. v. i., Prague
KIT	Karlsruhe Institute of Technology
LC	Liquid Chromatography
MEYS	Ministry of Education, Youth and Sport of the Czech Republic
MIT	Ministry of Industry and Trade of the Czech Republic
NMR	Nuclear Magnetic Resonance
NTA	Nitrilotriacetic Acid
PM	Particulate Matter
PolyHIPE	Porous Polymers from High Internal Phase Emulsions
POPs	Persistent Organic Pollutants
RAS	Russian Academy of Sciences
R&D	Research and Development
RFCS	Research Fund for Coal and Steel
SEM	Scanning Electron Microscope
TACR	Technology Agency of the Czech Republic
TU	Technical University
UCT	University of Chemistry and Technology
UJEP	Jan Evangelista Purkyně University in Ústí nad Labem, Czech Republic
UV	Ultraviolet
VOCs	Volatile Organic Compounds
VSB-TU	VSB - Technical University of Ostrava
VÚAnCh	Research Institute of Inorganic Chemistry, Inc., Ústí nad Labem
XRD	X-ray Diffraction

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