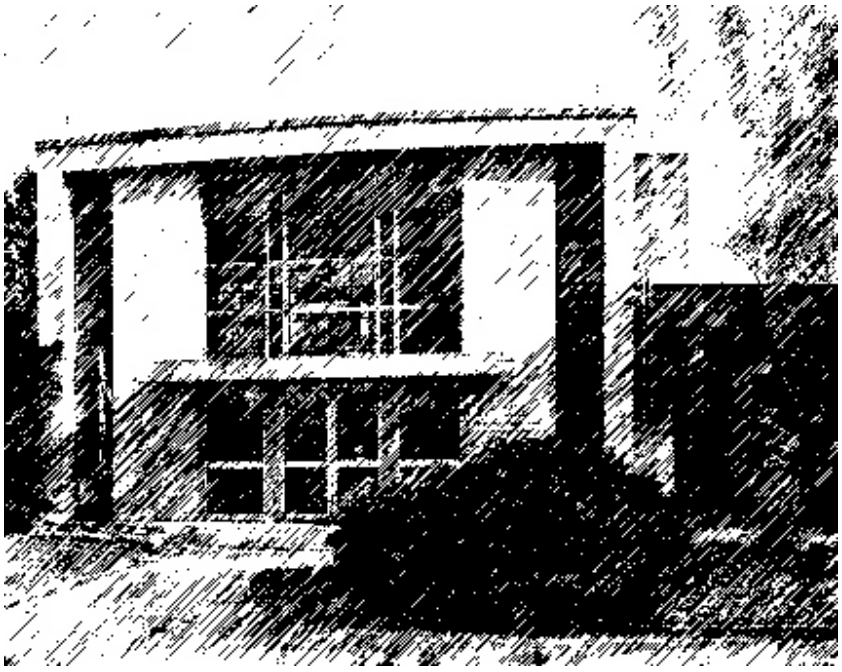
INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS OF THE CAS, V. V. I.

ANNUAL REPORT 2015

The Czech Academy of Sciences



ANNUAL REPORT 2015

Institute of Chemical Process Fundamentals of the CAS, v. v. i.
Prague 2016

ISBN 978-80-86186-79-5

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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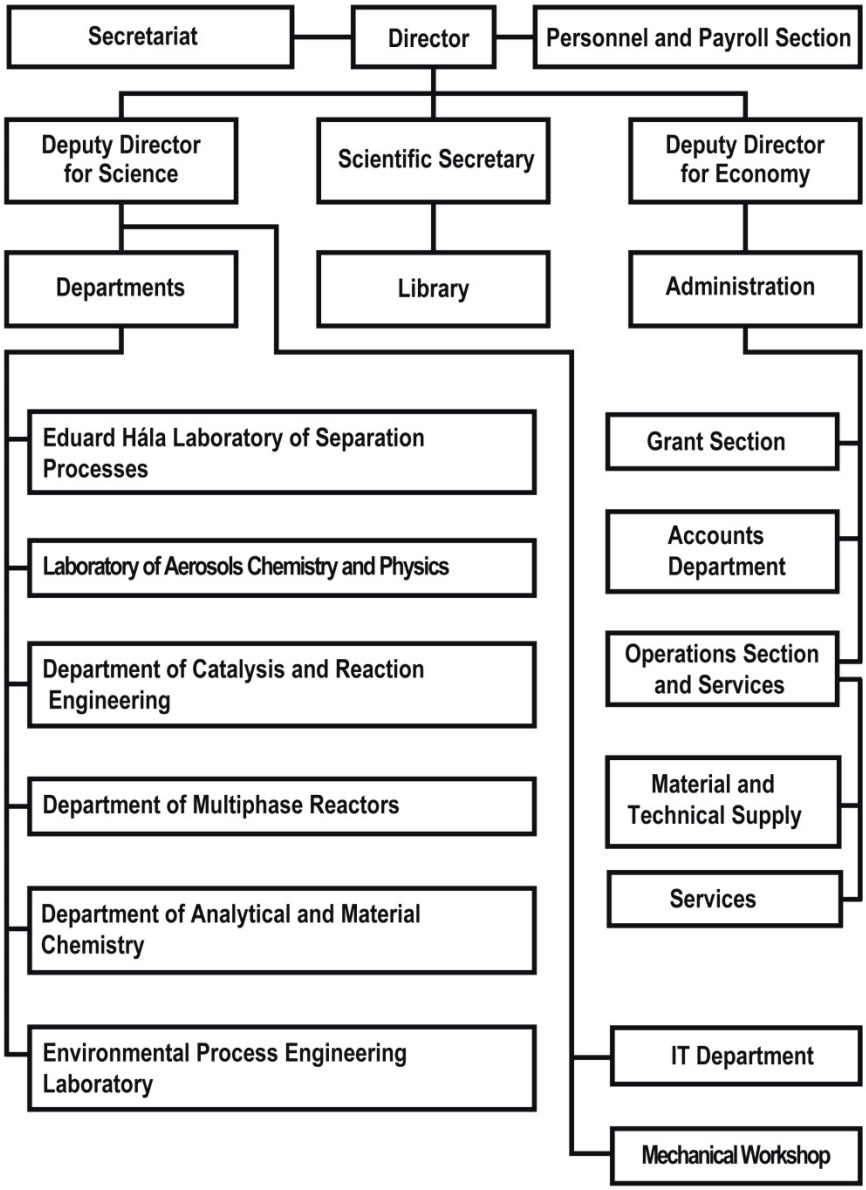
Organization Chart



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STAFF

(December 31, 2015)

Category	Number of Employees
Research	92
Research Support	70
Technical	11
Administrative	16
Services	10

BUDGET 2015

(24.60 CZK ≈ 1 US$, 27.28 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	62
Foreign R&D Funds and European Programs	12
Contracts with industry	8
Other resources	20
Total Resources	**177**

Expenses	Million CZK
Personal expenses including mandatory insurance	102
Purchase of material	19
Purchase of services	11
Repairs and maintenance	6
Depreciation of fixed assets	15
Travel expenses	4
Energy, water, and fuels	5
Total other expenses	9
Total other expenses	**171**

Profit	Million CZK
Total	**6**

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Main fields of research

- Thermodynamic properties and phase behavior of ionic liquids and their mixtures with molecular solvents
- Experimental determination of vapor –liquid equilibria in mixtures containing components of low and high molecular mass
- 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
- Separation of volatile organic compound from air
- Pertraction – separation of enantiomers
- 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
- Kinetic studies of hydrogenation reactions in a packed-bed microreactor
- Microreactors application for photosensitive reactions

- Methodology development for integration of 3D printing technologies in the advanced design, modelling and manufacture in chemical

Applied research

- Separation of unwanted components from raw biogas
- Separation of volatile organic compound from air
- Microtechnology application for kinetic studies and process intensification
- Utilization of microreactors as efficient tools for kinetic studies and process intensification
- Advanced separation methods developments for liquid-liquid systems

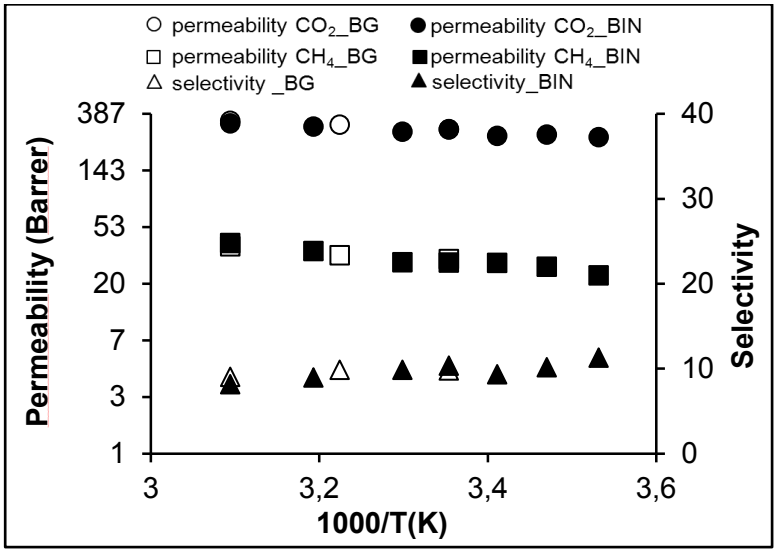
Research projects

Enrichment of raw biogas by methane

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

Membrane gas permeation found its place among the biogas upgrading methods some years ago. Here, we try to summarize the progress in the implementation of gas permeation in biogas upgrading. Gas permeation has been already accepted as a commercially feasible method for CO_2 removal. Many different membranes and membrane modules have been tested and also some commercial devices are available. On the other hand, utilization of gas permeation in other steps of biogas upgrading like desulfurization, drying, or VOC removal is still rather rare. This work shows that membrane gas permeation is able to compete with classical biogas upgrading methods and tries to point out the main challenges of the research.

The influence of the temperature and stage cut on permeation of CO_2 and CH_4 through two different supported ionic liquid membranes were studied (see Fig.). The measurements were performed with binary mixture of CH_4 and CO_2 and with real pre-dried biogas collected in sewage plant. The influence of temperature on permeability followed the Arrhenius behavior in agreement with solution diffusion model of transport. The influence of stage cut was also very small, what helped to confirm that the membrane was operated under optimal conditions. [Refs. 12, 39]



Temperature dependence of permeability and selectivity of CH_4 and CO_2 in binary mixture (denoted as BIN) and raw biogas (denoted as BG) in [emim][Tf_2N] membrane (permeability is displayed as a semilogarithmic plot) [Ref. 12]

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)

A different behavior of particular enantiomers was typically observed in the prepared membranes (although this behavior does not imply resolution of racemic mixtures in all cases) and hypotheses about the reason of these facts were formulated and published. The experimental results together with the mathematical description were also published in high impacted journals. Concerning new materials, we prepared large set of membranes based on

derivatives of saccharides and polyimides with covalently bonded chiral selectors or chiral secondary structure and membranes with chiral ionic liquid incorporated into the membrane.

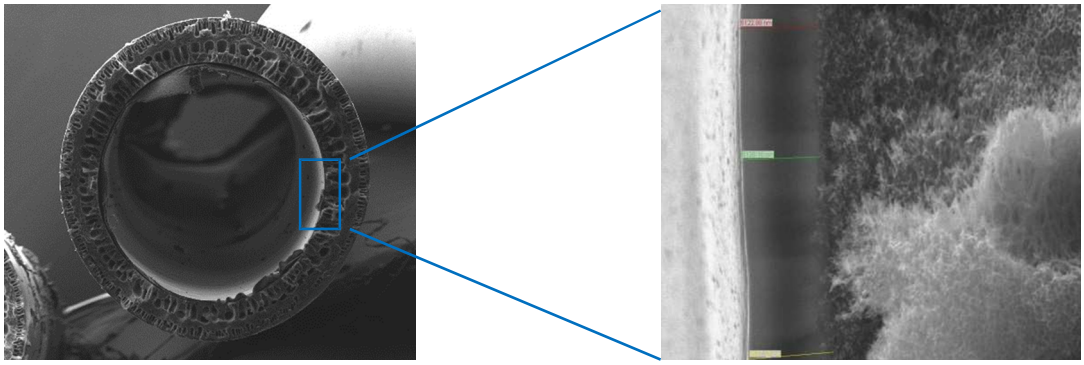
By our study, it was demonstrated that the supported chiral liquid membranes offer high selective solute transport which makes them particularly suitable for the recovery of minority solutes from complex mixtures, enantiomeric resolution and for the removal of specific contaminants from liquid or gas streams. We showed that these processes may be favored by the use supported ionic liquid membranes systems, since they allow better control of solute permeability and improved membrane stability by non-invasively modulation of magnetic ionic liquids viscosity and solubility by an external magnetic field. This aspect represents an important advantage for the optimization of small-scale processes commonly used in pharmaceutical industry. Our molecular simulations predicted a significant enhancement of the cation and anion densities at the interface in comparison with the liquid densities. In addition, the charge and atomic density profiles indicated that the vapor sides of interfaces are primarily populated by cation alkyl or chiral chains.

We considered possible patenting based on our results obtained within this basic research project. Also this project undoubtedly brought important findings in other related fields as physical and polymer chemistry, chemical engineering, and pharmacy. [Refs. 1, 2, 24, 36]

Separation of polar and non-polar gasses by membrane processes

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

Biogas upgrading is a widely studied and discussed topic. Many different technologies have been employed to obtain biomethane from biogas. Poly(ether-b-amide) (PEBAX 1657)/ polyacrylonitrile copolymer (PAN) composite hollow fiber membranes for potential use in CO_2/CH_4 separation were prepared by a new continuous coating method, referred to as cross-flow filtration. This technique allows obtaining the simultaneous coating of a large number of fibers, facilitating the scale-up. The dense layer was deposited in the lumen of the fibers allowing the coating of all the fibers in a single step. The coating on the inner surface of the fibers avoids the negative effects such as sticking or accidental mechanical damages occurring in the case of external coating. The membrane preparation was optimized by modulating different parameters. The optimal range of viscosity and concentration of the polymer solution to obtain a selective homogeneous PEBAX layer was identified. The presence of the PEBAX 1657 dense layer was confirmed by IR spectroscopy and the morphology of the composite membranes was observed by SEM analysis (see Fig.). Gas separation performance of the membrane modules was evaluated by single gas permeation measurements. A preliminary optimization yielded membranes with $P(CO_2)= 5*10^{-3}$ [m^3 m^{-2} h^{-1} bar^{-1}], $\alpha(CO_2/CH_4)$ = 18 equal to that of the neat dense polymer. The PEBAX/PAN hollow fibers modules are potentially useful for application in the biogas purification. [Refs. 5, 37, 39]

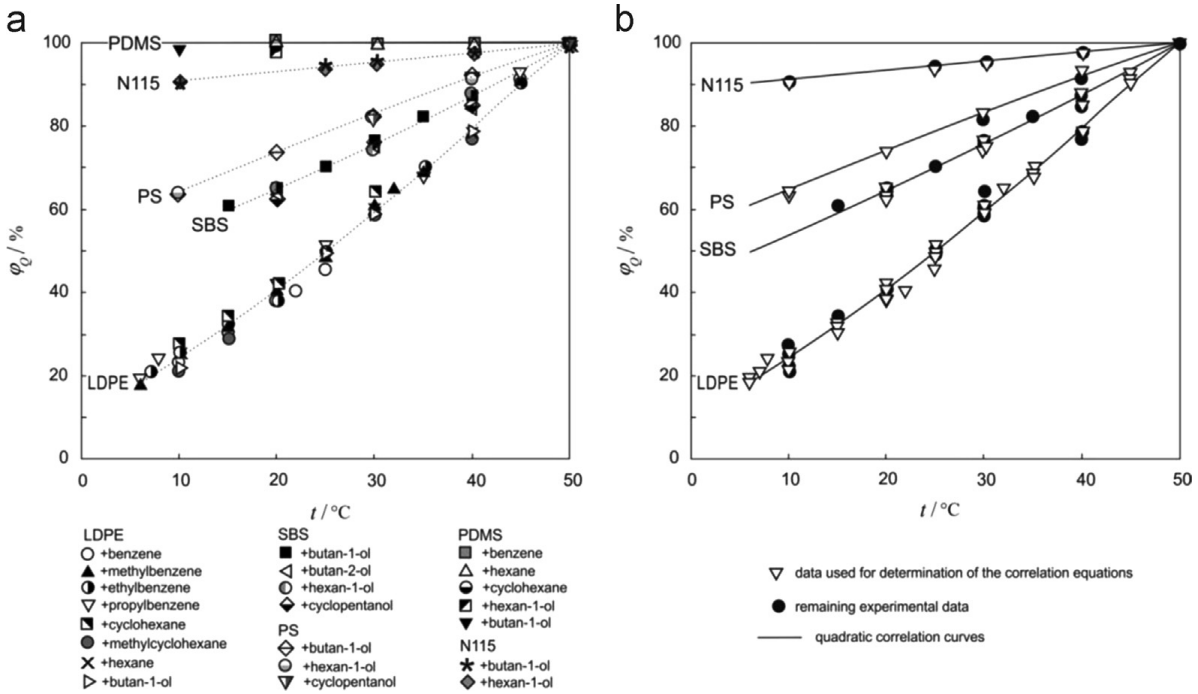


SEM images of the cross section of: composite hollow fiber membrane (left side); detail of the PEBAX coating layer on the inner surface (right side) [Ref. 5]

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 the project is the development of ionic-liquid containing membranes for the separation of volatile organic compounds and pollutants from flue gases. A new prediction method for sorption of low-molecular organic liquids (non-solvents) in polymers is presented (see Fig.). It was derived from the gravimetric data for sorption of linear and cyclic alkanes, aromatics and alcohols into various kinds of polymers (glassy polystyrene, rubbery polydimethylsiloxane, semi-crystalline low-density polyethylene, ion exchange Nafion, and copolymer poly(styrene-butadiene-styrene)) in temperature range 5-50 °C. [Refs. 21, 25, 35]



The normalized sorption values φ_Q as a function of temperature, (a) all experimental results, (b) quadratic polynomial correlation curves and experimental points divided into two groups: experimental data used for determination of the correlation equations (▽) and remaining experimental data for verification (●). Solid lines represent a prediction model while dashed lines serve as an eye guide only

Permeation of condensable gases trough asymmetric membranes

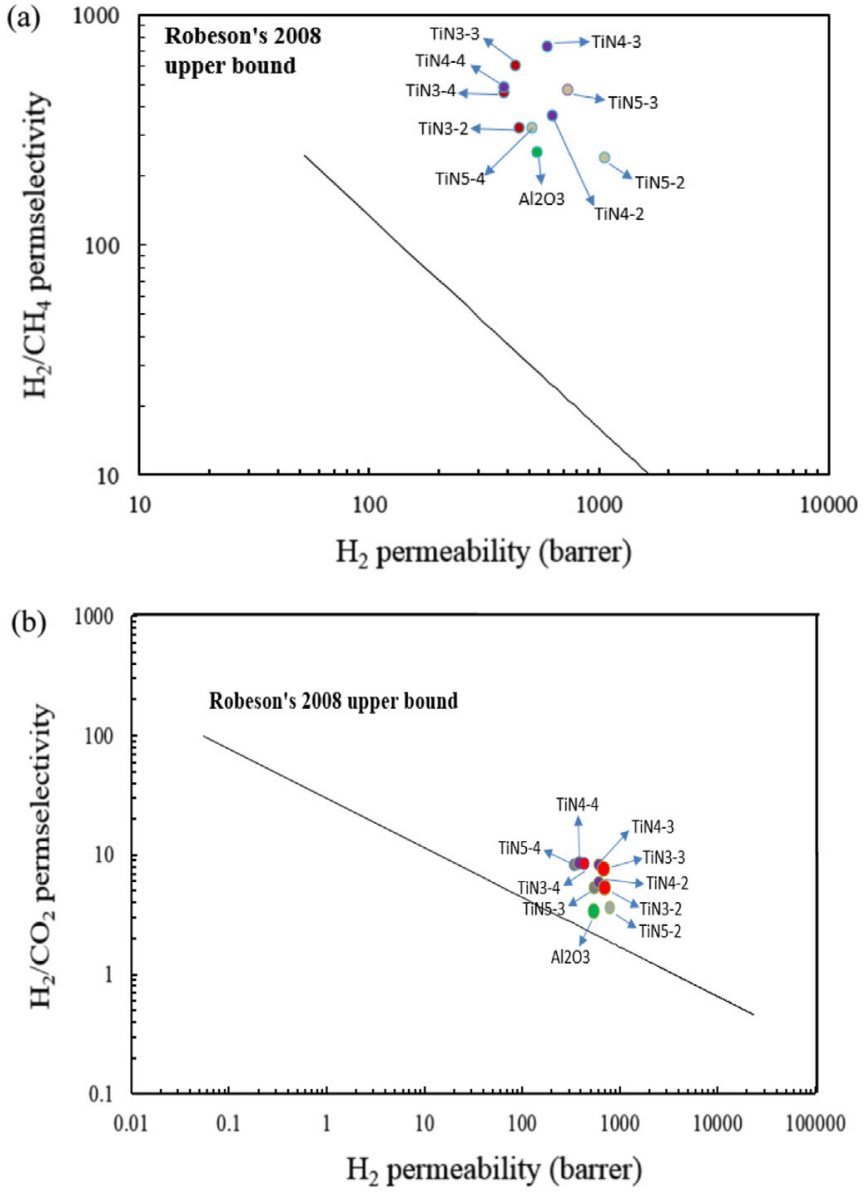
(J. Řezníčková, reznickova@icpf.cas.cz; joint project with Institut für Strömungsmechanik und Wärmeübertragung, Technische Universität Wien; supported by MEYS, MOBILITY, project No. 7AMB14AT011)

The aim of our collaboration is to carry out a series of experiments to obtain the pressure and temperature distributions within asymmetric ceramic membranes. Experimental data will improve our understanding of 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. 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 MOST/14/02)

Carbon/TiO_2/Al_2O_3 sandwich molecular sieving membrane synthesized via a sol-gel spin coating method followed by a carbonization process was proposed for the first time. Significantly influence on the adhesion mechanisms is observed from the TiO_2 intermediate layer coverage on an Al_2O_3 support and the microstructure and surface roughness of the TiO_2/Al_2O_3 composite support, whose fractions strongly depended on the sol-gel conditions, i.e., the molar ratio of HNO_3/TTIP and the number of coatings. Furthermore, to the best of our knowledge, the adhesion mechanisms of the CMS layer on the TiO_2/Al_2O_3 composite support were evaluated for the first time using EDX-line scanning, FTIR, and contact angle to determine the contribution from mechanical interlocking, chemical bonding, and adsorption, respectively. The results show that the three adhesion mechanisms might simultaneously contribute to the intrinsic adhesion depending on the preparation variables of the TiO_2 nano-network.



Performance of the TiO_2/Al_2O_3 supported CMS for the separation of (a) H_2/CH_4 and (b)CO_2/N_2 with respect to the Robeson trade-offline

CO_2/CH_4 separation by ionic liquid/polymer or composite membranes

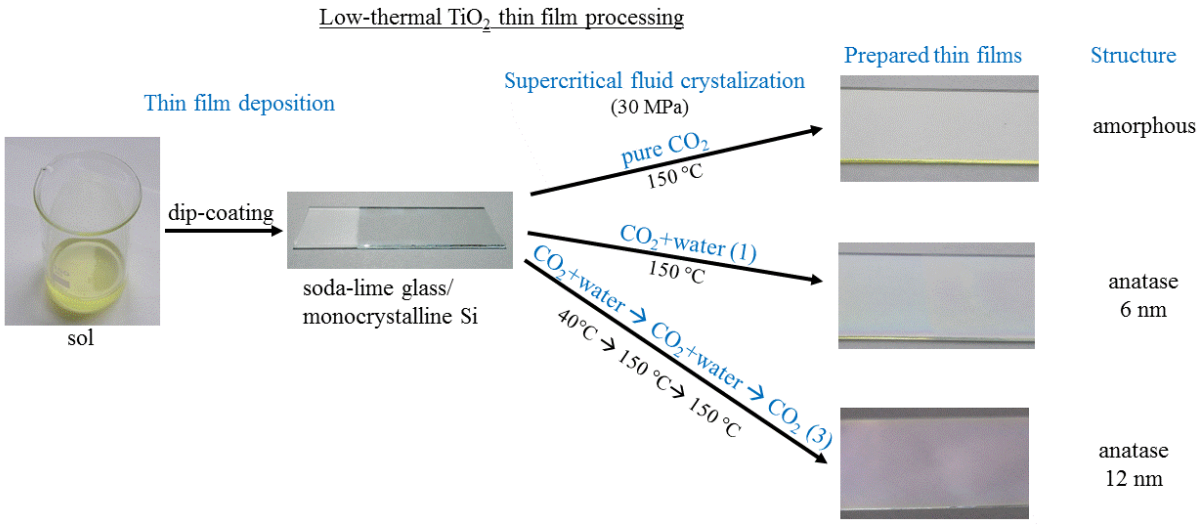
(K. Setničková, setnickova@icpf.cas.cz; joint project with Department of Chemical Engineering, National Chung Hsing University, Taiwan, supported by CAS, PPP project MOST/15/05)

Carbon dioxide is a major contributor to global warming. Significant efforts on decreasing CO_2 emission and increasing its recovery are undertaken all over the world. Membrane process is considered a promising technology for CO_2 recovery from gas mixture, and developing membranes with high CO_2 permeability and high separation factor becomes very important. Ionic liquid membrane is one of the candidates to achieve this goal. In most studies, ionic liquid is filled into the pores of a solid support. Gas permeation is accordingly affected by both the solid material and ionic liquid. It is suggested in this project by coating an ionic liquid layer upon a dense polymeric membrane with high CO_2 permeability to reduce the resistance on CO_2 permeation. Moreover, the combination of ionic liquid layer and dense membrane may enhance the overall gas selectivity. [Ref. 27]

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 concerns the direct preparation of highly pure nanocrystalline titanium thin films and aerogels by using supercritical fluids without any subsequent thermal treatment. The crystallization with pure and modified $scCO_2$ by water (5-30 wt. %) and/or organic solvent (10 wt. %) was tested. The temperature (40-150 °C), pressure (10-30 MPa) and the volume of CO_2 (50-200 g) passed through the extractor were optimized with respect to the microstructure and purity of TiO_2 thin films and aerogels. The purity and crystallinity of prepared TiO_2 thin films and aerogels were estimated by Raman spectroscopy. The crystallite size and the phase composition were determined by X-ray diffraction. Textural properties of aerogels such as the surface area and the pore-size distribution were characterized by nitrogen physisorption and helium pycnometry measurements.



Morphology evolution of nano- and micro-cellular polymeric foams

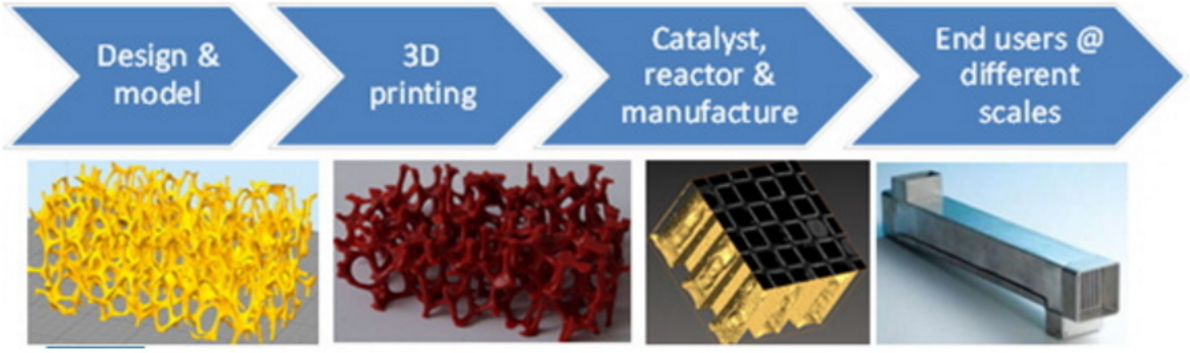
(H. Sovová, sovova@icpf.cas.cz; joint project with Faculty of Chemical Engineering, UCT Prague and New Technology – Research Centre, University of West Bohemia, supported by GACR, project No. GA14-18938S)

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.

Process intensification through adaptable catalytic reactors made by 3D printing (PRINTCR3DIT)

(P. Stavárek, stavarek@icpf.cas.cz; EC Horizon 2020, project: 680414, www.printcr3dit.eu)

PRINTCR3DIT is a joint effort between world-leading industries (4), innovative SMEs (4), R&D institutes (4) and a university that aim to accelerate deployment of a set of products to the market. The project is coordinated by SINTEF Materials & Chemistry, Norway. The main objective of the PRINTCR3DIT project is to implement a methodology to integrate 3D printing in the advanced design, modelling and manufacture of structured catalysts and catalytic reactors with significant cost reductions, access to new design strategies and faster lead times.



The principal target of the project is to increase the efficiency through process intensification in reactions that present heat, mass and momentum transfer limitations, with targeted goals to significantly reduce the energy consumption, increased selectivity and longer lifetimes. The utility and flexibility of the methodology will be demonstrated through three industrial processes that span different chemical sectors, scales of production and catalytic reactors. The selected examples will target the production of fine chemicals, commodity chemicals and fertilizers.

Development of advanced separation methods for liquid-liquid systems

(P. Stavárek, stavarek@icpf.cas.cz; research contract with Modelarna LIAZ s.r.o.)

The research activities on the topic of advanced separation methods for mixtures of miscible liquids continued well on basis of results gained from previous cooperation. The efforts were focused on experimental validation and optimization of the methods with a constructed laboratory apparatus. The collected results were documented and critically evaluated in three confidential research reports.

Application of microreactors for gas phase catalytic reactions

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

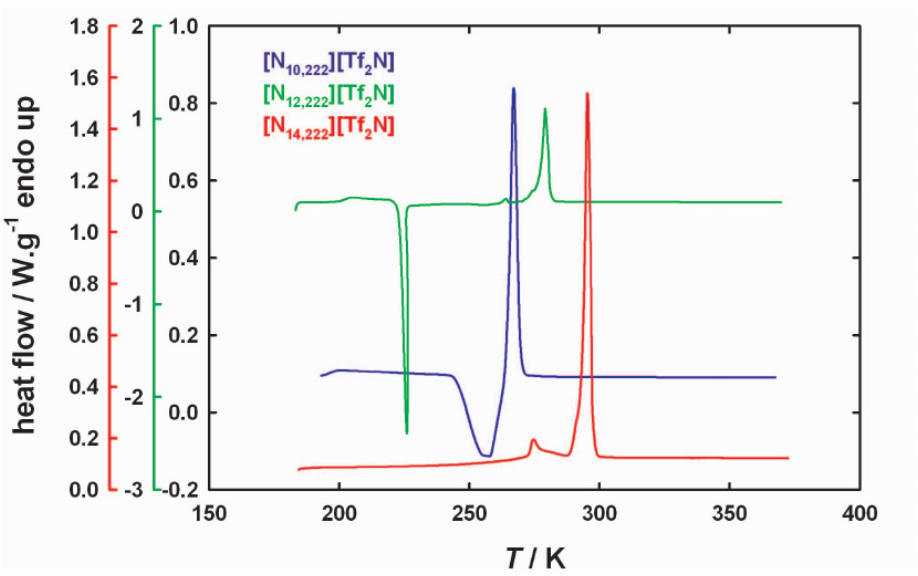
Well established cooperation with Hexion a.s. continued with systematic research of microreactors and their application to gas phase catalytic reactions. As the microreactor design was completed in previous project stages the efforts were now focused on the microreactor construction and its assembling, laboratory apparatus design and analytical

method development to analyze products of a case study reaction. The analytical method was successfully developed, experimentally validated and quantified with participation of one diploma thesis student. Next project stage is the laboratory testing with a case study reaction.

Thermal properties of alkyltriethylammonium bis(trifluoromethyl)sulfonylimide ionic liquids

(M. Bendová, bendova@icpf.cas.cz; joint project with J. Jacquemin of QUILL Belfast, UK)

Thermal properties, phase and glass transition behavior, of selected members of a homologous series of alkyltriethylammonium bis(trifluoromethyl)sulfonylimide, i.e. [$N_{R,222}$][Tf_2N], ionic liquids were studied using differential scanning calorimetry (DSC). Decomposition temperature was also determined in the present series by thermal gravimetry analysis. Furthermore, isobaric molar heat capacity as a function of temperature for hexyltriethylammonium, octyltriethylammonium, and dodecyltriethylammonium bis(trifluoromethyl)-sulfonylimide ionic liquids. Based on the data obtained, we discuss the influence of the alkyl chain length of the cation on the studied ionic liquids on the measured properties. Using viscosity data obtained in a previous work, the liquid fragility of the ionic liquids is then discussed. Viscosity data were correlated by the VTF equation using a robust regression along a gnostic influence function. In this way, more reliable VTF model parameters were obtained than in our previous work and a good estimate of liquid fragility of ionic liquids was made.

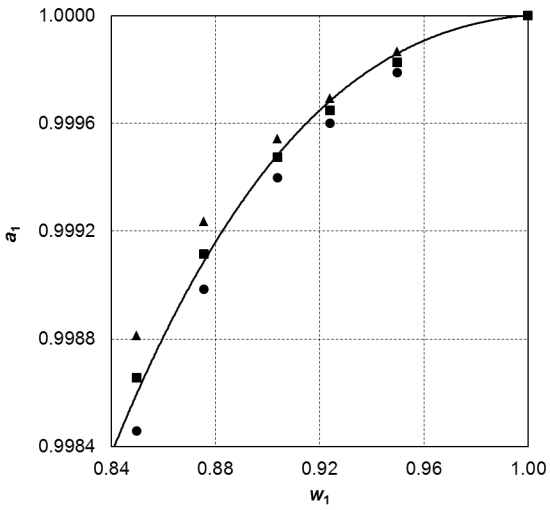


Comparison of solid-liquid and solid-solid phase transitions for [$N_{R,222}$][Tf_2N] ionic liquids where R stands for decyl, dodecyl, and tetradecyl [19]

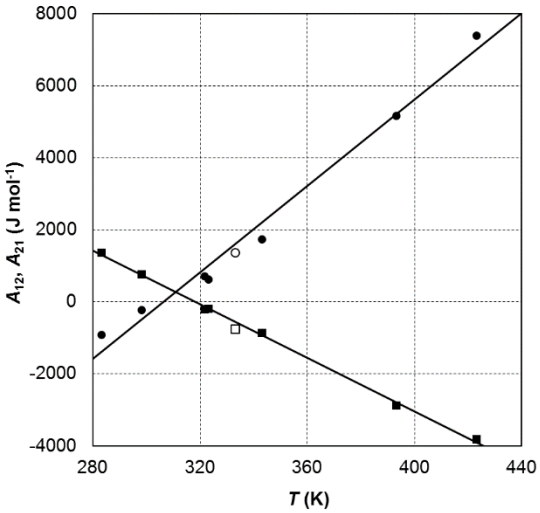
Thermodynamics of polymer solutions: experiments meet theory and vice versa

(I. Wichterle, wi@icpf.cas.cz; supported by GACR, project No. 15-19542S)

Experiments: Vapor-liquid equilibria have been determined in systems composed of polystyrene + toluene [Ref. 22], and polystyrene + butan-2-one [Fluid Phase Equilibria, in press] by ebulliometric method, i.e. by total pressure measurement. The ebulliometer has been redesigned in 2014 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. Results were presented at two international conferences, too.



Activity a_1 of butan-2-one in PS as a function of butan-2-one weight fraction w_1. Experimental data at (●) 323.15 K, (■) 333.15 K and (▲) 343.15 K. Solid line represents predicted activities at 333.15 K using the UNIQUAC-FV parameters estimated using all data within temperature range 323.15–343.15 K.



Temperature dependence of UNIQUAC-FV A_{12} (■) and A_{21} (●) parameters. Open points represent UNIQUAC-FV parameters evaluated from our data at 323.15–343.15 K and plotted at mean temperature 333.15 K.

Theory: The first year study was aimed to electrolytes since ions are present in every solution. The complete description of solution is at hand if chemical potential is known. The calculation of chemical potential via molecular simulation is complicated and moreover existing data are not in mutual agreement even for simple systems. However, all the proofs have testified that our simulations are well working. Two papers by other scientists presented in 2015 have confirmed correctness of our (the best in the world) computations. This result has been published at 5 international meeting and prof. Nezbeda was invited to prepare the perspective review dedicated to this project for Molecular Physics journal, which was submitted in December 2015.

The problems of polymer self-assembly in relation to phase equilibria (solid/liquid and liquid/vapor interfaces) were studied. Experimental investigation of the co-assembly of block copolymers with surfactants has been performed. The extensive manuscript deals with the electrostatic co-assembly of polymeric micelles with surfactants by a combination of a number of experimental techniques. Even though it is aimed mainly on the structure of formed nanoparticles and on the mechanisms of underlying processes, it shows that some fluids components of the studied polymer–colloid–solvent mixtures are engaged in non-volatile complexes and do not contribute to the vapor–liquid equilibria.

Other activities: High-pressure phase equilibrium data in the carbon dioxide + 1-chloropropane binary system were published [Ref. 11]. As guest editors, we prepared a special issue of the Chemical and Biochemical Engineering Quarterly with contributions from 21st CHISA Congress [Ref. 40].

International co-operations

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

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

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, Max-Planck-Institut für Dynamik-komplexer technischer Systeme, Magdeburg, Germany: 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

Queen's University Belfast, QUILL: Database on liquid-liquid equilibria of binary mixtures of ionic and molecular compounds, IUPAC Project #2011-065-3-500

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

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 lanthanides

Wrocław University of Technology, Faculty of Chemistry: Physicochemical characterization of chiral ionic liquids based on a natural terpene substituent

J. Hanika: UCT, Faculty of Chemical Technology, postgradual course “Multiphase Reactors”

H. Sovová: UT Maribor and Graz UT, The European Summer School in High Pressure Technology

M. Bendová: UCT, Faculty of Chemical Engineering, postgraduate course “Physical Chemistry for Technological Practice”

M. Bendová: UCT, Faculty of Chemical Engineering, postgraduate course “Introduction into irreversible thermodynamics: theory and practice”

Z. Sedláková: UJEP, Faculty of Science, courses for under-graduated students “Membrane Separations”, “Basic of Chemistry”, “Physical chemistry”, “Experimental and Nonexperimental methods in Physical Chemistry”

Awards

Hanika J. – Hanuš Memorial Medal, 2015, for the merits for the development of chemistry, from the Czech Chemical Society

Hanika J. – Annual Prize 2015, for the merits for the development of chemical reaction engineering, from the Czech Society of Chemical Engineering

Publications

Original papers

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tamate) Selective Layers for Separation of Toluene - *n*-Heptane Mixtures. *J. Membrane Sci.* 477, 14-24 (2015).

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Patents

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Laboratory of Aerosols Chemistry and Physics

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DEPUTY
MARTIN LÍSAL

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Main fields of research

- Atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- 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

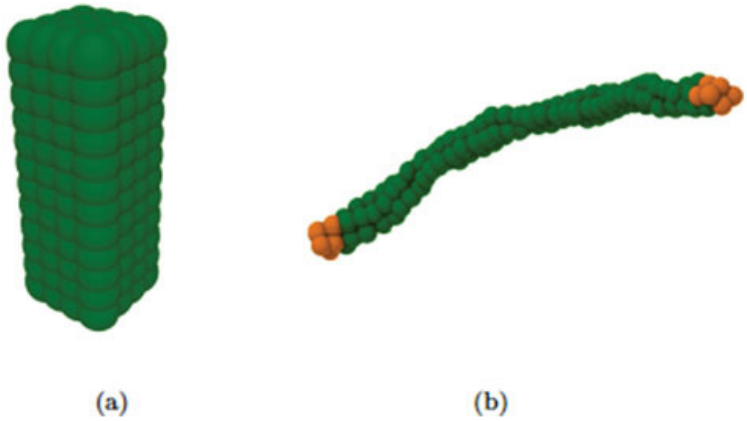
(I. Nezbeda, ivonez@icpf.cas.cz; joint project with the University of Ontario, Institute of Technology, Oshawa, ON, Canada and UJEP; supported by UJEP)

This project 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. 11, 15, 24, 27]



Schematic of the meso-scale models: (a) parallepepid model P with 192 *p*-type beads (green) and (b) elongated model L with 136 *p*-type beads and 16 *k*-type beads (orange)

A controlling of diffusion processes in pores with varying permeability

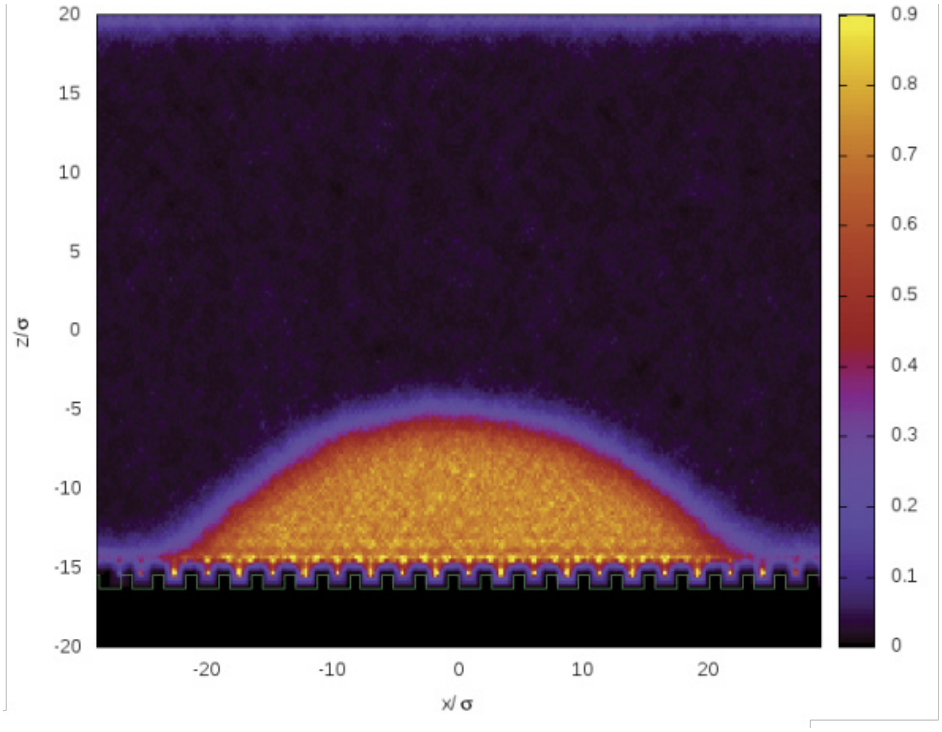
(A. Malijevský, M. Lísal, malijevsky@icpf.cas.cz, lisal@icpf.cas.cz; supported by GACR, project No. 13-09914S)

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. 16, 17]

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. 11, 17]



Two-dimensional density profile of liquid droplet on the molecularly rough surface

Maximizing the EU shale gas potential by minimizing its environmental footprint (ShaleXenvironmenT)

(M. Lísal, lisal@icpf.cas.cz; supported by EU HORIZON2020, project No. 640979)

Securing abundant, affordable, and clean energy remains a critical scientific challenge. Fortuitously, large shale formations occur within Europe. As the conventional gas production in Europe peaked in 2004, European shale gas could become a practical necessity for the next 50 years. However, the exploitation of shale gas remains challenging. Further, its environmental footprint is at present poorly quantified. Great care is needed to assess and pursue this energy resource in the safest possible way for the long-term future of Europe whilst protecting the European diverse natural environment.

With this in mind, ShaleXenvironmenT assembled a multi-disciplinary academic team, with strong industrial connections. The primary objective is to assess the environmental footprint of shale gas exploitation in Europe in terms of water usage and contamination, induced seismicity, and fugitive emissions. Using synergistically experiments and modeling activities, ShaleXenvironmenT will achieve its objective via a fundamental understanding of rock-fluid interactions, fluid transport, and fracture initiation and propagation, via technological innovations obtained in collaboration with industry, and via improvements on characterization tools. ShaleXenvironmenT will maintain a transparent discussion with all stakeholders, including the public, and will suggest ideas for approaches on managing shale

gas exploitation, impacts and risks in Europe, and eventually worldwide. The research will bring economical benefits for consultancy companies, service industry, and oil and gas conglomerates. The realization of shale gas potential in Europe is expected to contribute clean energy for, e.g., the renaissance of the manufacturing industry.

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)

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. [Refs. 2, 5, 6]

Aerosols, Clouds, and Trace gases Research InfraStructure Network

(V. Ždímal, zdimal@icpf.cas.cz; supported by EC, project No. INFRA-2010-1.1.16 ACTRIS)

ACTRIS (Aerosols, Clouds, and Trace gases Research InfraStructure Network) is the 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”.

Aerosols, Clouds, and Trace gases Research InfraStructure Network

(V. Ždímal, zdimal@icpf.cas.cz; supported by EU HORIZON 2020, project No. 654109, ACTRIS-2 IA)

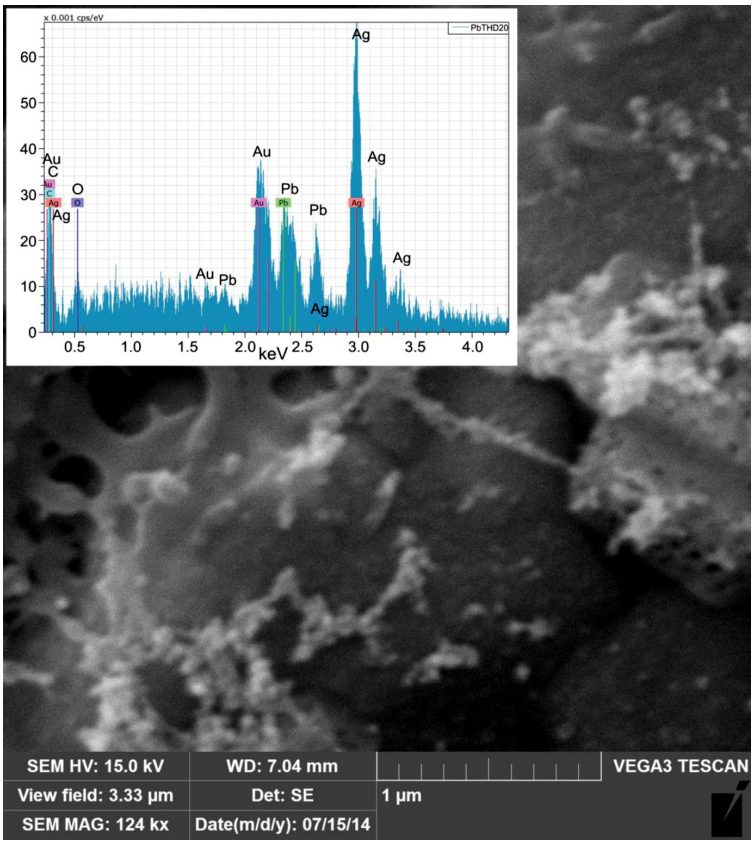
Detecting changes and trends in atmospheric composition and understanding their impact on the stratosphere and upper troposphere is necessary for establishing the scientific links and feedbacks between climate change and atmospheric composition. The primary objective of ACTRIS is to provide the 4D-variability of clouds and of the physical, optical and chemical properties of short-lived atmospheric species, from the surface throughout the troposphere to the stratosphere, with the required level of precision, coherence and integration. The second objective is to provide effective access to this information and the means to more efficiently use the complex and multi-scale ACTRIS parameters serving a vast community of users working on models, satellite retrievals, and analysis and forecast systems. The third objective is to raise the level of technology used in the RI and the quality of services offered to the

community of users, involving partners from the private sector. Finally, the fourth objective of ACTRIS is to promote training of operators and users and enhance the linkage between research, education and innovation in the field of atmospheric science.

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. [Refs. 10, 13, 22, 23]



SEM image and EDS spectrum of the sample of NPs synthesized by oxidation of PbTHD2 at T_R = 480 °C, Q_R = 1400 cm^3/min, P_{PbTHD2} = 2.20 Pa, and c_O = 5 vol. %

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 depen-

dences between damage of library and archival collections and surrounding environment, leading to precautions reducing the adverse effects of deteriorated environment. [Refs. 1, 9]

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: Source apportionment from highly time-resolved data.
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behavior
Technical University of Crete, Chania, Greece: Aerosols in the indoor environment
Technical University of Denmark, Lyngby, Denmark: Indoor air and aerosols
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. Cusack: University of Birmingham, Birmingham, UK (1 month)
A. Malijevský: Imperial College London, London, UK (1 month)
N. Talbot: IDAEA- CSIC, Barcelona, Spain (3 months)
N. Zíková: Clarkson University, NY, U.S.A. (5 months)

Publications

Original papers

[1] Benešová M., Mašková L.: Mechanické čištění papíru a certifikovaná metodika "Metodika výběru prostředku k mechanickému čištění prachových částic z povrchu papíru". (Czech) The Mechanical Cleaning of Paper and the Certified Methodology "Methodology of the Selection of an Agent for the Mechanical Cleaning of Dust Particles from the Surface of Paper". *Archivní časopis* 65(4), 358-373 (2015).

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Main 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 nanofibrous membranes and catalytic supports
- Assymetric Hydrogenations with Chiral Complexes in Ionic Liquids
- Advanced Hydrogen Storage Media

Applied research

- Catalytic combustion of volatile organic compounds
- Advanced oxidation processes for environment
- Textural characteristics of structural materials
- Green chemistry for biomass utilization to the high added-value products
- Enhancement of the power transformer operation security and failure prevention
- Decontamination of brownfields contaminated by organic compounds and heavy metals

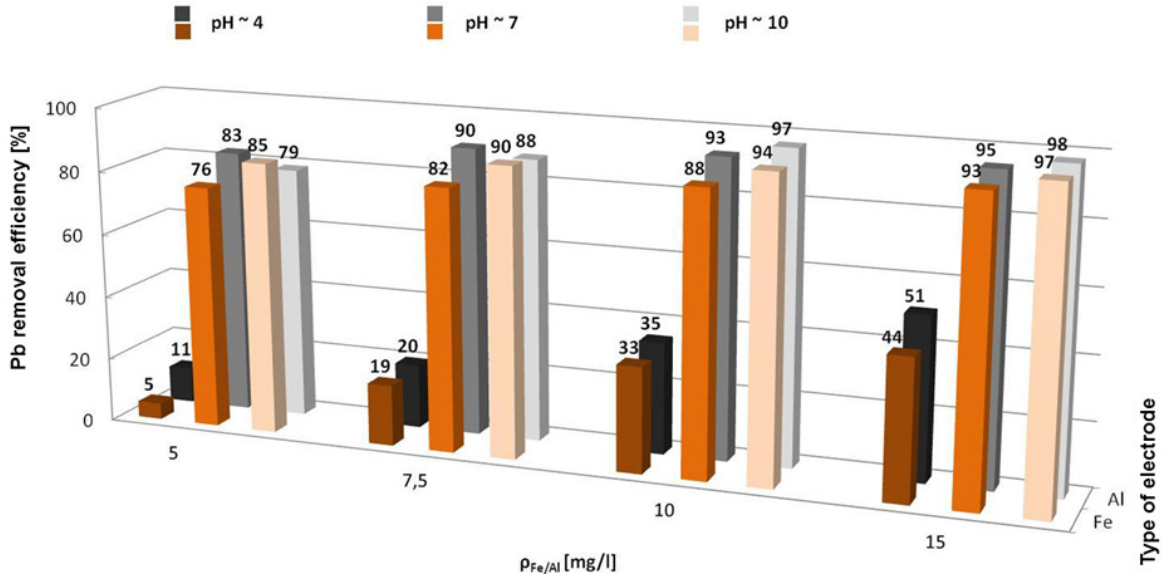
Research projects

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. 5]



Influence of initial pH on Pb removal efficiency

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)

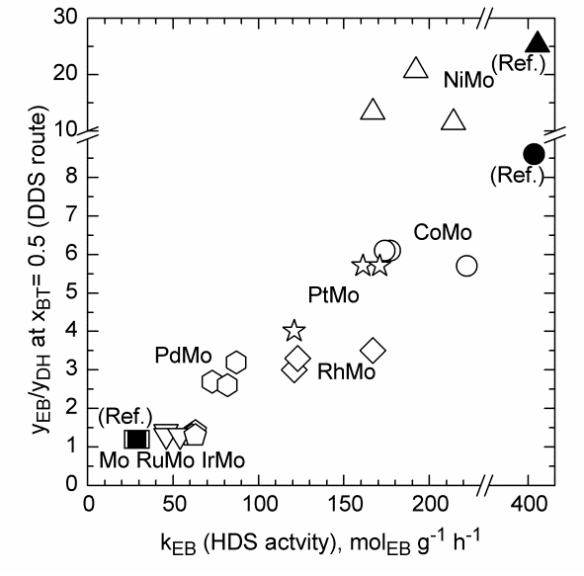
Catalysts were successfully prepared from five different experimental carbon blacks by impregnation with hexachloroplatinic acid, calcination, reduction and dechlorination. Calcination has been found to greatly increase the electrochemical stability. Dechlorination resulted in a 1.1–1.7-fold increase of the Pt crystallites, but did not alter the S_{BET}. Furthermore, the electroactive surface area (ESA) did not change significantly upon dechlorination, indicating that the purification and rearrangement taking place during the

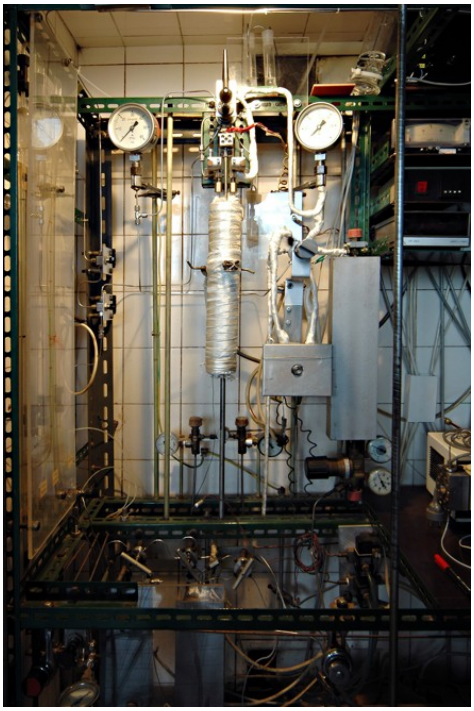
dechlorination procedure are beneficial in terms of electrochemical utilization of the Pt. The prepared catalysts exhibited similar ESA of about 30 m^2 g_{Pt}^{-1}, and all showed higher specific electrocatalytic activities toward the ORR than that of the commercial high-surface-area reference catalyst of S_{BET} = 359 m^2 g^{-1}, while their mass-specific ORR activities were slightly lower. All five catalysts showed better electrochemical stability of the support than the reference, which shows the benefit of using a support with moderate surface area. The stability of the Pt particles was better than the reference for one of the catalysts, namely Pt/CB3. This catalyst also had the highest S_{BET} (193 m^2 g^{-1}), the smallest Pt particles (6.1 nm), the best mass-specific ORR activity (31 A g_{Pt}^{-1}) and the lowest residual Cl content (1380 ppm). It could be concluded that the high S_{BET} of CB3 within the moderate-surface-area CB supports is by far the most critical parameter influencing ESA and electrochemical stability. Catalyst manufacture based on the carbon type with large graphitic domains (CB5) was found to result in catalysts that perform poorly in terms of activities. [Refs. 12, 36]

Unconventional composition and preparation of sulfide hydrotreating catalysts

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

The 1-methyl-cyclohexene hydrogenation (o-HYD) was studied with 1-benzothiophene hydrodesulfurization (HDS) over Co, Ni, Mo, W, Rh, Re, Pd, Pt, Ir, CoMo, NiMo, RhMo, ReMo, PdMo, PtMo, IrMo supported catalysts. The CoMo/MgO catalysts exhibited at least 3.3-fold activities but the same selectivity C=C hydrogenation/C-S hydrogenolysis as the reference industrial CoMo/Al_2O_3catalyst. Furthermore, mesoporous silica-aluminas (MSA) of different composition were studied as supports of Pd-Pt catalysts in transformation of refractory 4,6-dimethyldibenzothiophene (4,6-DMDBT). Activities of majority of Pd-Pt catalysts correlated with their Brønsted acidities. Pd-Pt/MSA catalysts were much more active than a conventional sulfide catalyst; the loadings around 0.10 wt. % gave 5-7 time more active catalysts than CoMo/Al_2O_3. [Refs. 10, 11, 30, 37]



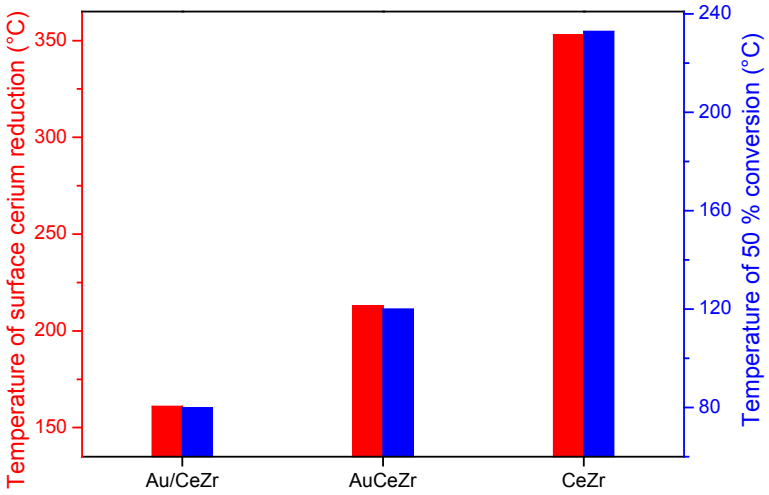


Correlation of relative selectivity direct desulfurization/hydrogenation desulfurization (DDS/HYD, y_{EB}/y_{DHBT} at x_{BT} = 0.5) and overall HDS activity (k_{EB}) in hydrodesulfurizaion (HDS) of 1-benzothiophene over zirconina supported catalysts in laboratory tubular flow microreactor

Washcoated ceramic monoliths for total oxidation of volatile organic compounds

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

The innovative monolithic catalysts based on noble metals (platinum, palladium, gold) supported on electrospun nanofibre mats or on ceria-zirconia mixed oxide were studied. It was shown that except the type of noble metal, the key properties of the catalyst are noble metal loading and particle size, and that these properties depend on the method of catalyst preparation. By employing a proper preparation method, required physicochemical characteristics of the catalyst, especially reducibility and acidity, can be reached. Such catalysts then exhibit high activity and/or selectivity in the investigated reaction. However, it was also demonstrated that activity and selectivity of a given catalyst strongly depend on the type of volatile organic compound. Therefore, tailored synthesis of a catalyst is needed to achieve such combination of reducibility, acidity and resistance to poisoning, which would be suitable for a studied pollutant. The obtained results were published in impacted international journals. [Ref. 26]



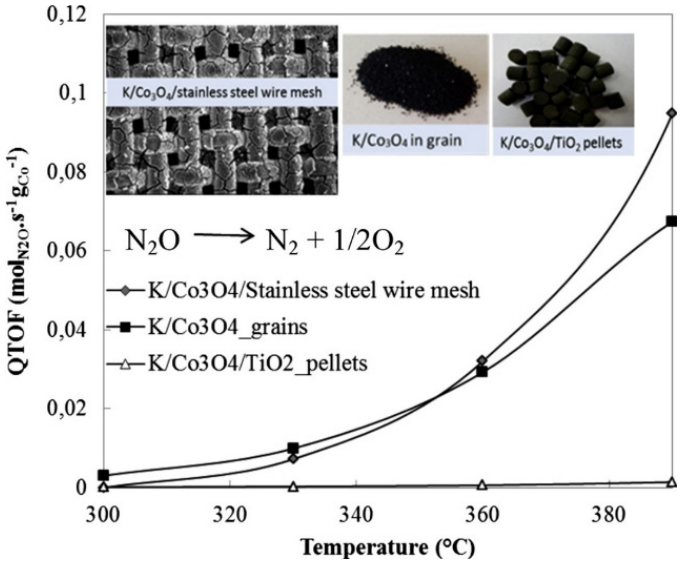
Correlation between reducibility of ceria-zirconia based catalysts and their performance in the elimination of model volatile organic compound (ethanol)

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)

Supported Co_3O_4 catalysts were prepared by heating of the cobalt hydroxide synthesized electrochemically on stainless steel sieves and by heating of the commercial TiO_2 pellets impregnated with cobalt nitrate solution. Mathematic simulation results showed that higher conversions in potential large scale application can be achieved over the catalyst deposited on stainless steel sieves in comparison with TiO_2 pellets. A significant increase in catalytic activity with increasing amount of cesium promoter was observed without respect to the Cs precursor.

Ethanol total oxidation over mixed oxide catalysts containing various transition metal cations was studied. The M^{II}-M^{III} layered double hydroxide (LDH) precursors with M^{II}/M^{III} molar ratio of 2 (M^{II} = Cu, Co,Ni, Cu-Ni, Cu-Co, and Co-Ni; M^{III} = Mn or Al) were prepared. The ternary mixed oxides containing Mn were more active than the binary Cu-Mn, Co-Mn, and Ni-Mn ones as well as the ternary Al-containing catalysts; the Cu-Co-Mn and Cu-Ni-Mn mixed oxides were the most active. The catalytic activity increased with increasing amount of easily reducible components and amount of oxygen desorbed from catalysts surface at lower temperatures (up to 500◦C). [Refs. 8, 9, 15, 22, 37]



Influence of various catalysts on their efficiency

Assymetric Hydrogenations with Chiral Complexes in Ionic Liquids - Reaction Engineering Aspects

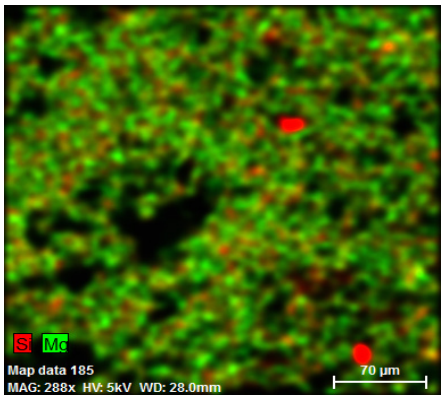
(P. Klusoň, kluson@icpf.cas.cz; supported by GACR, project No. 15-04790S)

In 2015 interactions of the catalytic Ru-BINAP complex with an inorganic matrix were studied and evaluated with help of XPS study. A detailed XPS study of interactions of [RuCl((*R*)-binap)(*p*-cymene)]Cl catalytic complex with Montmorillonite as characteristic type of inorganic support upon employing various types of immobilisation approaches was performed. This complex is typically used for stereoselective hydrogenations of β-ketosteres. It was shown that XPS is a method well suited for studying interactions of the Ru complex immobilised onto an inorganic matrix, either directly or via a heteropolyacid spacer. It informed on the surface stoichiometry, surface elemental composition, and energetic differences in the nearest vicinity of the main surveyed bonded elements. The interaction of Ru complex with an inorganic matrix via the heteropolyacid spacer is usually referred to as of covalent nature. Here it was shown that it was not at least clearly evident. The work could be understood as a model case study for many similar systems. The interaction of the catalytic Ru-BINAP complex with the model surface of Montmorillonite depends very much on the chosen method of immobilisation. The chemical form of the Ru complex plays also a certain role. Some effect of the used type of heteropolyacid was identified as well. For the Ru-BINAP complex either immobilised or in its standard crystal form there were no significant differences of the binding energies. On the other hand a shift towards higher E_B values for the dimer complex MDM was evident. Fort Ru-BINAP immobilised directly onto the Montmorillonite surface an increase of a binding energy appeared likely due to its interaction with an electronegative substituent. [Refs. 1, 2, 27, 31, 34]

Combined sorption modes for energy storage

(O. Šolcová, solcova@icpf.cas.cz; supported by GACR, project No. 15-14228S)

The project "Advanced Hydrogen Storage Media - Combined Sorption Modes" focuses on the design and preparation of high capacity sorbents for hydrogen storage via combination of chemisorption and physisorption processes. The first year of the project duration the major works within the task devoted to hydrogen storage assessment (based on determination of high-pressure adsorption isotherms of hydrogen and hydrolysis of silicides) were focused mainly on preparation and characterization of nanostructure materials (TiO_2, ZnO) including dopants based on sol-gel technique. [Refs. 3, 4, 6, 21]

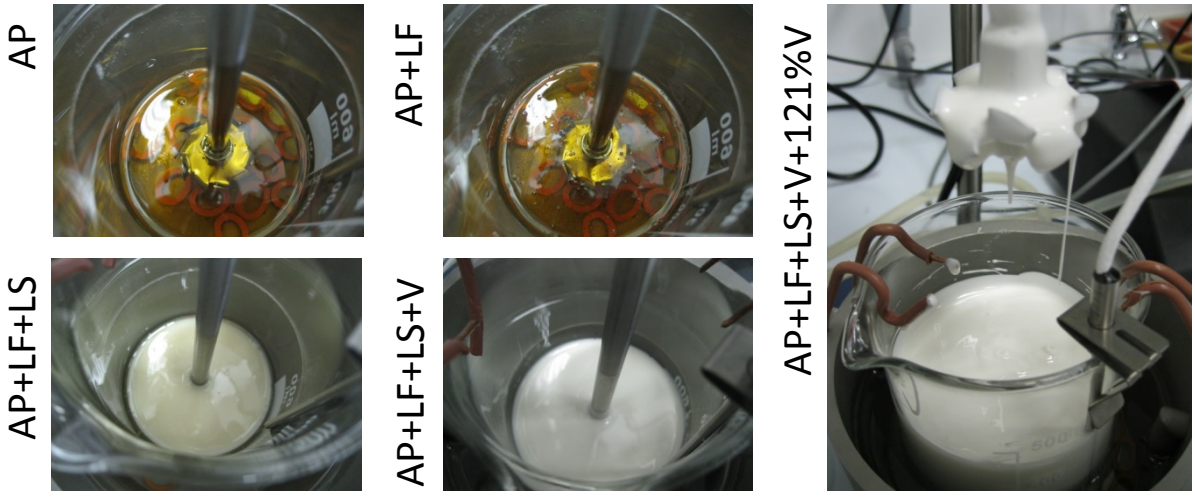


Prepared magnesium silicides by EDX

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

(P. Klusoň, kluson@icpf.cas.cz; joint project with Teluria, TECHEM CZ; 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.



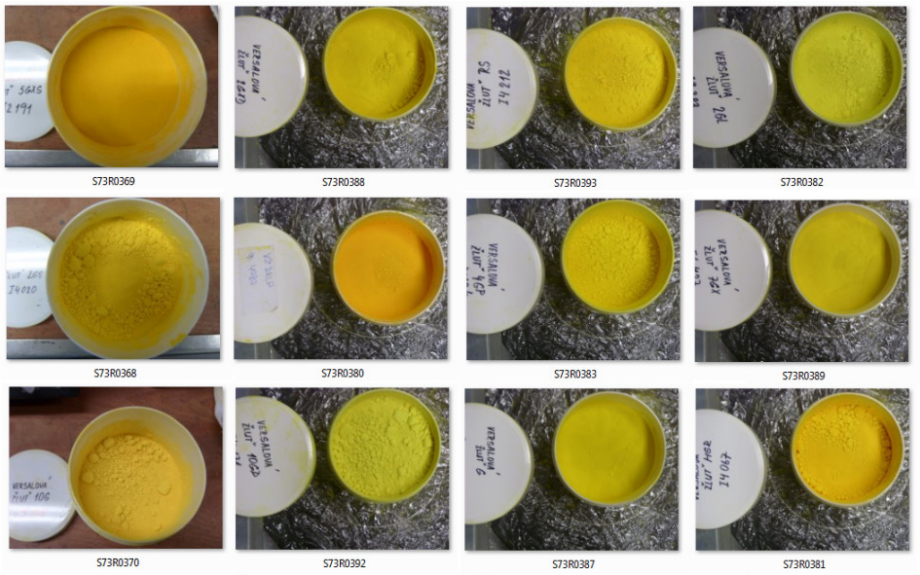
Emulsification progress with and without special additives

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. 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 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 ($N_{R,222}Tf_2N$, R = 6, 7, 8, 10, 12, 14) with a variable length of an alkyl chain are specially promising.



Differences of various pigment granulation

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)

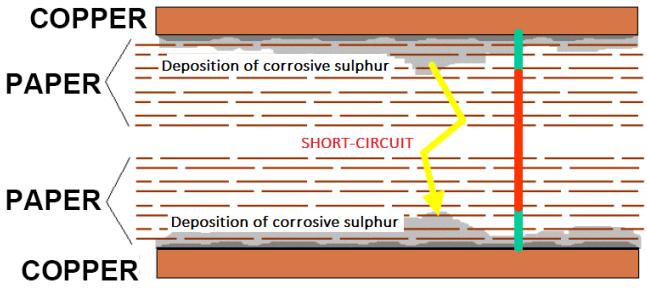
In 2015 the detection system entitled Colour Clocks, and supported by the Technology Agency of the Czech Republic TACR, was successfully completed. Two types of light sensitive and preciously calibrated dosimeters were brought to the production level at the cooperation company Invos Ltd. The first dosimeter was denoted as the Gallery one. It is supposed to be used as part of strategies to protect valuable museum, archive and galleries artefacts. Light is generally known as one of the most critical factors to such items. It monitors the light exposure, and the recorded values could be than used to plan/limit future expositions, way of conservation, storage, transportation etc. Comparable systems are usually very expensive, based on sophisticated electronic devices, and requiring complicated technical equipment/support, and experienced operation, periodical control etc. The second system is denoted as the Derma-Clock, or as Derma dosimeter. Here, the target group is represented by standard users who seek of effective prevention when sunbathing. The high risk resulting from the exposure of the human skin to UV light from sun is generally known. It indicates, in the dependence of the skin sensitivity, the level of safe sun-light exposure, at different light conditions. It could be also corrected according to the applied sun protection factor of the used sunscreen cream. [Refs. 23, 24, 39, 40]

The first presentation of dosimeters to the public at the festival Night of Science, Brno, September 2015

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. [Refs. 14, 29]



Generating of short circuit

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)

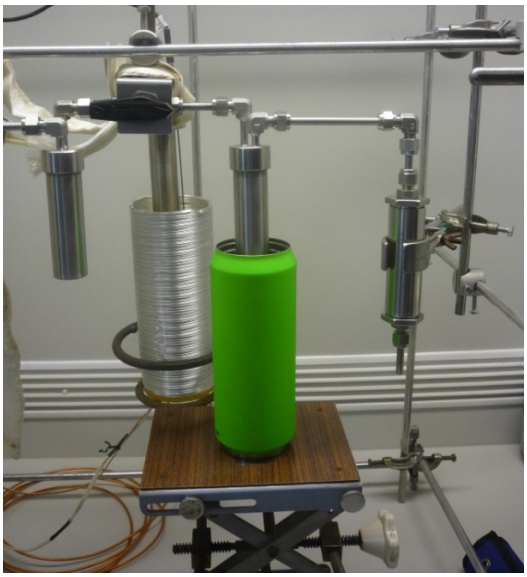
The project is focused on utilization of the lipid new sources with the high content of the healthy polyunsaturated fatty acids (PUFAs), omega-3 types. Microorganisms, mainly bio-technologically produced eustigmatofit microalgaes with the high content of PUFA, have been applied. New types of mixotrophic bioreactors were designed to obtain the optimal content PUFA in biomass. Products will be used as the feeding additives for poultry. [Ref. 17]

The newly designed mixotrophyreactor

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 separation 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 with. [Refs. 13, 19, 20, 25, 28]



Stainless steel laboratory thermal desorption apparatus

Electrochemical removal of toxic metals from polluted water

(P. Kluson, kluson@icpf.cas.cz; supported by TACR, project No. TA04020130)

The aim of the project "Electrochemical removal of toxic metals from polluted waters" is aplication of electrocoagulation method with following pilot scale testing on the treatment of industrially polluted waters. These waters contain dissolved metallic ions – especially ions of toxic elements (Cr^{III+}, Cr^{VI+}, As^{III+}, As^{V+}, Cu^{II+}, Cd^{II+}, Pb^{II+}, Co^{II+}, Ni^{II+}, V^{III+}, V^{V+}, Zn^{II+}, Al^{III+}). The attention will also be paid to removal of other noble metallic ions (e.g. Eu, Gd, Y, Yb) coming from electro-technical industry (compact fluorescent lamps, LCD panels, diodes, photovoltaic panels etc.).

The electrocoagulation technology has a great potential especially for treatment of specific waters coming from electro-technical industry with low concentrations of noble lanthanide and actinide group metals that can be after separation process returned back to the production process. That enables not only the industrial production frugality but also the production cost savings in consideration of price of these metals. Another broad area of application can be found in wastewater treatment coming from chemical, metallurgical, engineering or printing industrial sector. [Refs. 16, 18, 35, 38]

Electrocoagulation set-up

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)

Al_2O_3-CeO_2 supports containing 1-10 wt% Ce were prepared mechanochemically by milling aluminum and/or cerium nitrates with NH_4HCO_3. Heteropolymolybdate, $(NH_4)_4NiMo_6O_{24}$, was used as the precursor of the Ni and Mo to prepare $NiMo_6/Al_2O_3$-CeO_2 components in catalysts by impregnation method. The physicochemical properties of the catalysts were determined using chemical analysis, X-ray diffraction, temperature-programmed H_2 reduction, temperature-programmed NH_3 desorption, X-ray photoelectron spectroscopy (XPS), and the Brunauer-Emmett-Teller method. The catalyst acidity decreased with increasing Ce concentration in the support. XPS showed that the NiS/MoS ratio decreased two-fold for the Ce-modified alumina support. $NiMo_6/Al_2O_3$, which had the highest acidity, showed the highest activity in hydrodesulfurization of 1-benzothiophene (normalized per weight of catalyst). The concentration of surface MoO_xS_y species (which is equal to the concentration of Mo^{5+}) gradually decreased to zero for catalysts with Ce concentrations higher or equal to 10 wt. %. However, the activities of all the catalysts prepared mechano-chemically from Al_2O_3 and Al_2O_3-CeO_2 supports significantly exceeded that of a reference $NiMo_6/Al_2O_3$ catalyst prepared by impregnation method using the same precursor and with the same composition.

International co-operations

National University of Engineering, Lima, Peru: Determination of transport properties of the adobe brick building materials
University of Tumbes, Peru: Preparation and utilization of activated carbons prerpared from agro-forestry biomass waste materials
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: Chemical bonding in solids
University of Oulu, Oulu, Finland: New catalysts for VOC oxidation and Hybrid membrane processes 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
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
University of Maribor, Maribor, Slovenia: PolyHYPE polymers
University of Barcelona, Barcelona, Spain: Ion exchanger catalysts
Zhejiang University, Hangzhou, China: Mesoporous poly(divinylbenzenes)
University of Bangor, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials
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

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Department of Multiphase Reactors

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Main fields of research

- Dynamics of gas-liquid, gas-liquid-solid and solid-fluid mixtures (experiments and numerical simulations)
- Effect of surface active agents on the multiphase systems
- Bubble/drop breakup and coalescence phenomena
- Complex rheology of microdispersions, powders and granular mixtures
- Flow of gas-liquid dispersions in channels and microchannels
- Hydroacoustic detection of bubbles in shallow water reservoirs
- Stability and behavior of complex beverage foams

Research projects

Bubble break-up in a turbulent flow

(J. Vejražka, vejrazka@icpf.cas.cz, supported by GACR, project No. 15-15467S)

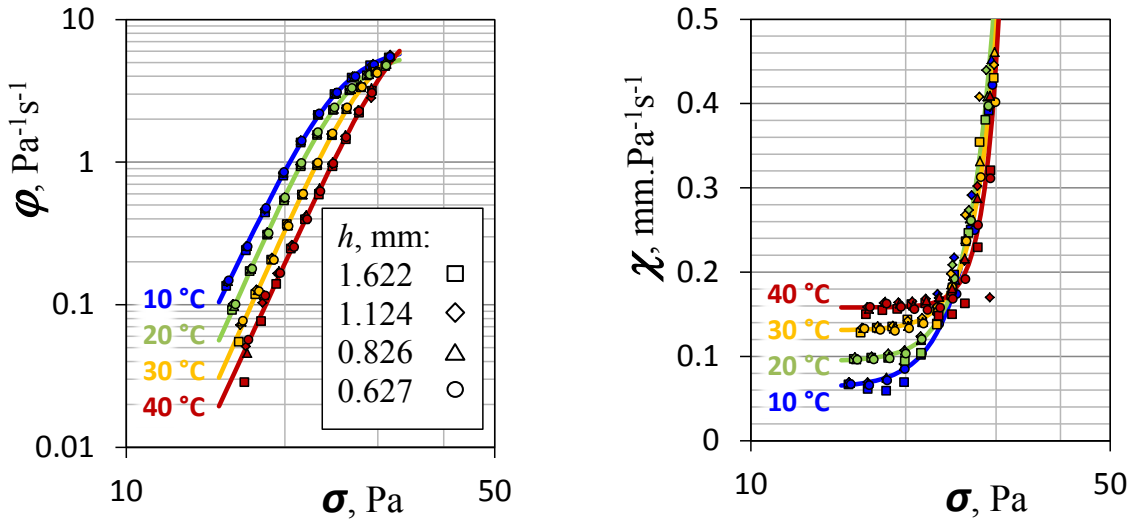
In frame of proposed project, breakup of fluid particles (bubbles and drops) in a turbulent liquid flow is studied. The probability of particle breakup and size distribution of daughter particles is established. It will be tested how the breakup process is affected by presence of surfactants in the system. Experiments are carried out in a channel, in which turbulent energy can be controlled. Velocity field and turbulence characteristics are measured using PIV. The particle breakup is recorded by means of high-speed camera. The experiment allows determining the breakup frequency and the size distribution of daughter particles in dependence on local mean shear, turbulence properties (ε, two-point cross-correlations) and on properties of bubble or drop interface. The final result should be the validation of current models for particle breakup or a new model, useable as breakup kernel in Population Blance Modelling (PBM) simulations.

Visualization of break-up sequence of a bubble in an experimental turbulent channel

Interface transport phenomena in microdisperse liquids

(V. Pěnkavová, J. Tihon, O. Wein, penkavova@icpf.cas.cz, supported by ICPF)

Flow of microdisperse liquids along a solid wall can be accompanied by the flow anomaly in proximity of the wall called apparent wall slip (AWS). Experimental detection of AWS effects is possible by performing a series of viscometry measurements over the same range of shear stresses in sensors with different gap thicknesses. These measurements must be executed precisely and a proper data treatment must be made to evaluate flow and slip functions reliably. A parametrical study of aqueous kaolin suspensions are made, where the fluidity and slip functions are obtained from the results of AWS viscometry. This parametrical study covers wide range of the kaolin concentration, temperature and surface quality of used sensors. The influence of deflocculating electrolytes, which are used for increasing flow-ability of kaolin suspension, is also studied. [Refs. 9, 13]

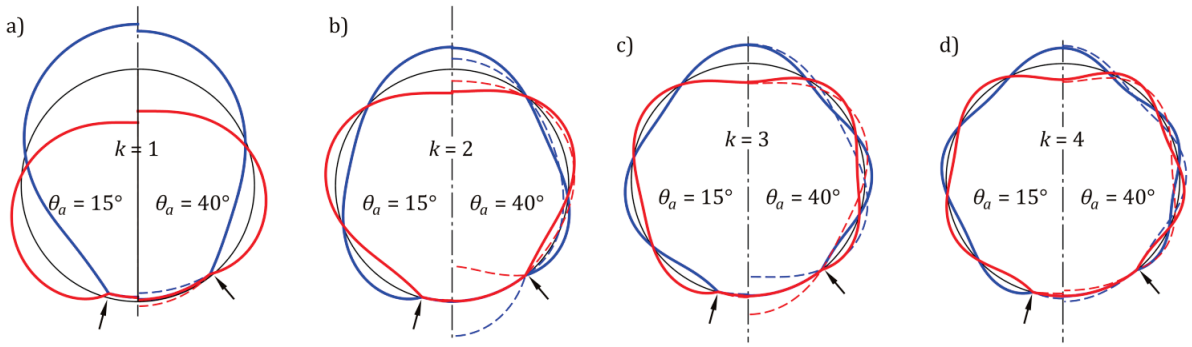


Fluidity φ and slip χ material functions evaluated for 30% aqueous kaolin suspension in sensor made from stainless steel with smooth surfaces at different temperatures. σ corresponds to applied shear stress, the legend inform about gap thickness h during measurement

Properties of the phase interface – their measurement and their influence on the behavior of macroscopic flows

(J. Vejražka, S. Orvalho, vejrazka@icpf.cas.cz, international project COST, Smart and Green Interfaces, also supported by MŠMT, project No. MP1106)

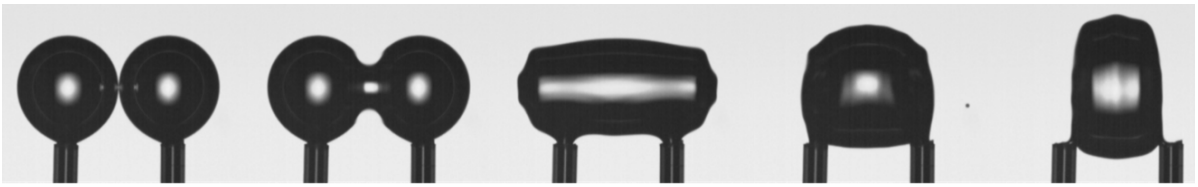
The project aims to improve methods used for characterization of phase interfaces, and further to deepen the knowledge about the interface properties links to the behavior of macroscopic systems. Specifically a methodology for determination of the phase interface properties is developed, based on the evaluation of the shape oscillations of bubbles and drops. [Ref. 5]



Shape of the first four eigenmodes of a pinned bubble. Left halves of figures represent attachment angle θ = 15°, right halves of figures are for θ = 40°. The attachment positions are indicated by arrows. Solid lines are for the Strani & Sabbeta constraint, dashed lines are for the Bostwick & Steen constraint. Blue and red lines correspond to positive and negative displacement of the interface at the apex, respectively

A devices with small channel instrumented with wall-mounted electrodiffusion sensors for diagnostics of multiphase flows in small channels is developed. Further, the effect of surfactants and electrolytes on the coalescence probability of bubbles and droplets is studied. The relation between dynamic parameters (bubble approach velocities, liquid viscosity) and

bubble coalescence probability is found [Ref. 8]. Last but not least, the behavior of foams in dependence on interfaces properties is studied in order to clarify the stability of the beverage foams. [Ref. 7]

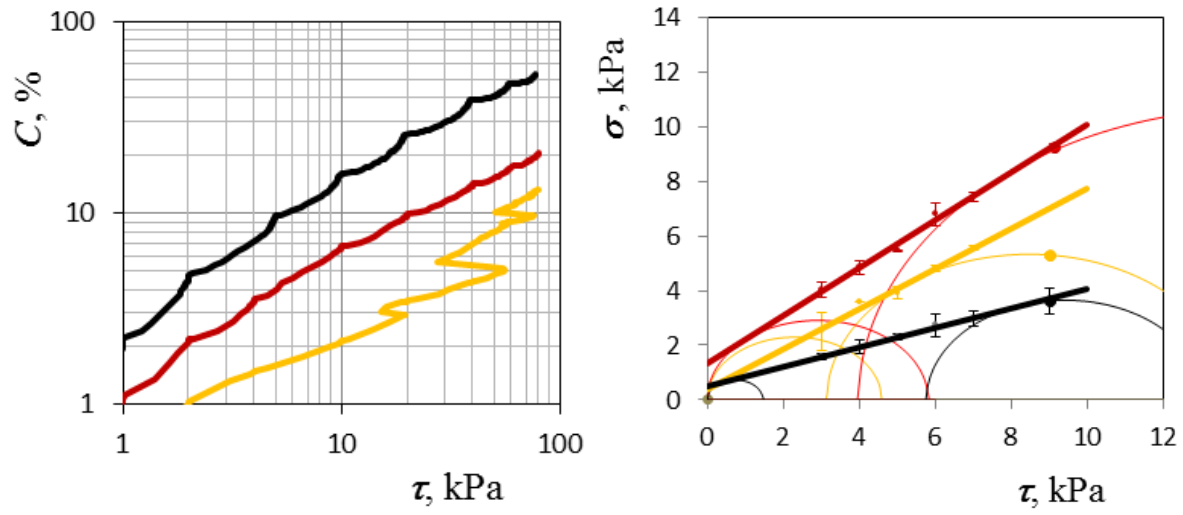


The bubbles synchronously grow on the capillaries till they touch. It marks the end of the inflation interval and the beginning of the contact time interval. Eventually, the bubbles either coalesce or detach from the capillaries separately [Ref. 8]

Structure-property relationships and breakage dynamics of complex granular material

(M. Růžička, M. Punčochář, V. Pěnkavová, L. Kulaviak, ruzicka@icpf.cas.cz, penkavova@icpf.cas.cz, supported by GACR, project No. 15-05534S)

A granular material in the form of a layer of particles or granules with a complex internal structure is common in many engineering applications. As compressive and shear stress field is applied, the material undergoes structural changes associated with deformation, breakage, and particle rearrangement within the layer. The present understanding of the link between primary particles properties, applied stress field, and the structure evolution, is mostly based on empirical knowledge only. The proposed research project consists of Discrete Element Method (DEM) simulation of different scenarios, where a granular material is subjected to stress field. For a subset of suitable scenarios, measurements in powder rheometer will be carried out in parallel with the simulations to verify their validity. An extensive data set generated by both the simulations and the experiments will be analyzed in a search for fundamental principles and relations describing granular material structure evolution.

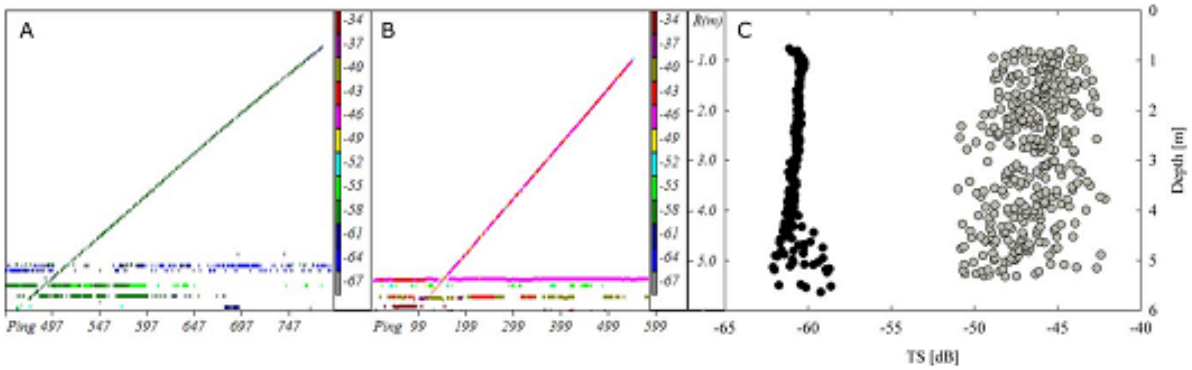


Compressibility C and shear stress σ in dependence on applied normal stress τ measured using powder rheometer FT4 for three different granular materials with needle-like shaped particles. High compressibility and low friction are exhibited by the elastic material (glass fibres – black lines), less compressibility and the highest friction are exhibited by cohesive material (terephtalic acid – red lines), and the fractures on compressibility curve and high friction exhibit the breakable material (rod-like pasta – yellow lines)

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 method for estimation of methane ebullition from bottom sediments of shallow freshwaters was subject of presented research. Artificially prepared methane bubbles of various sizes were released from a bottom in a freshwater reservoir. An acoustic target strength (TS) of these bubbles was measured using both the vertical and horizontal beams of a 120 kHz frequency split-beam sonar used by fisheries. Relationship of the mean TS variation with bubble volume was obtained in both modes of observation. Further, TS distribution around mean value was presented as well and its width and shape was discussed in relation to the bubble path and change of bubble size during rise. TS changes during rise for both the vertical and horizontal mode of observation was within the range of standard deviation of TS measurement and model for dissolution have shown that gas exchange is compensated by expansion of bubble during rise. Hence depth effect could be neglected for evaluation of acoustic target strength regression models used in shallow waters down to 6m. [Ref. 2]

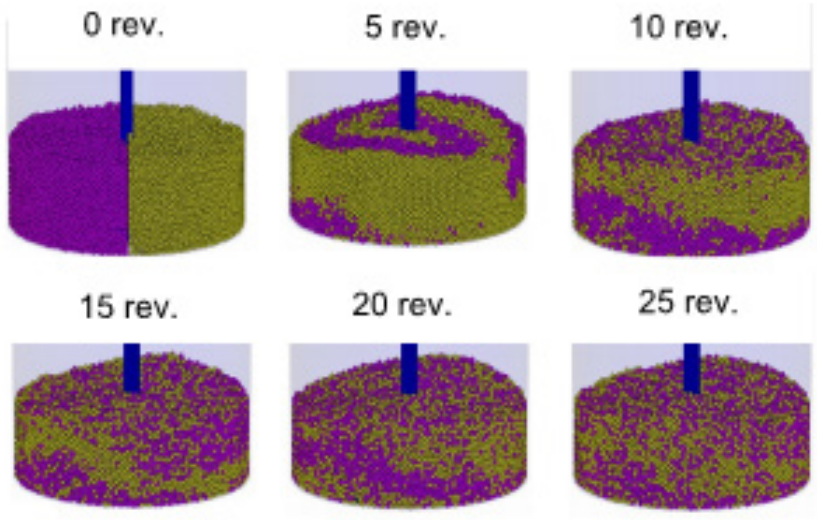


Echograms depicting a rising single bubble with initial size (A) D = 1.7 mm and (B) D = 9.8 mm from vertical acoustic observation. The (C) is chart of their acoustic target strength (dB) depending on depth, black dots mark bubble A and grey ones bubble B

Hydro-mechanical interactions of particles in solid-fluid systems

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

The behavior of granular media has been studied for a long time, due to their omnipresence and practical importance (rocks, soil, sand, cement, coal, food materials, technology media, pharmaceutical powders, etc.). Granular media are after water the second most widely used material in human activities. Many industries, such as agriculture, food processing, constructional, chemical or pharmaceutical, use granular materials on a large scale. From the physical point of view, granular materials are complex systems, whose are governed by mutual interactions. These interactions have crucial importance for prediction of flow behavior in process apparatuses or for correct design of industrial technologies. The main objective of this project is to suggest physical concepts for describing dynamical behavior of granular systems and suspensions. These concepts will be used for describing global macroscopic characteristics of unit chemical engineering operations. In the project we focus especially on the mixing of granular material, the process of the particle settling and fluid flow through the settled substrates. We expect that the project will bring important original results of description of granular system behavior. [Refs. 1, 4]



Snapshots of mixed granular bed initially radially divided into two halves with differently colored particles for the first 25 revolutions. The blade rotational speed is 15 rpm

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, bubble/drop breakup

Centre de Recherché et de Transfert de Technologies, Saint Nazaire, France: Microfluidics

Aristotle University of Thessaloniki, Thessaloniki, Greece: Microfluidics

Manufacturing and Process Technologies Research Division, University of Nottingham, United Kingdom: Experimental diagnostics in gas-liquid flows, bubble columns

Università degli Studi di Napoli Federico II., Italy: Bubble coalescence, effect of surfactants on flow in bubble columns

Publications

Original papers

[1] Barczi T., Trávníčková T., Havlica J., Kohout M.: Effect of Bed Depth on Granular Flow and Homogenization in a Vertical Bladed Mixer via Discrete Element Method. *Chem. Eng. Technol.* 38(7), 1195–1202 (2015).

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[3] Hadač O., Kohout M., Havlica J., Schreiber I.: Oscillations and Patterns in a Model of Simultaneous CO and C_2H_2 Oxidation and NO_x Reduction in a Cross-Flow Reactor. *Phys. Chem. Chem. Phys.* 17(9), 6458-6469 (2015).

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Patents

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Main fields of research

- Chiral separation of helicenes
- Determination on $^{n}J(^{13}C\text{-}^{13}C)$ coupling constants
- Fluorous organocatalysis
- Carbosilane dendrimers in bioapplications
- Antitumor properties and mechanism of action of metallocenes modified by carbohydrate or heterocyclic substituents
- Synthesis of helicene derivatives and [*n*]phenacene derivatives
- Sensors based on laser ablated graphene
- Silicon nanowires grown on metal substrates

Applied research

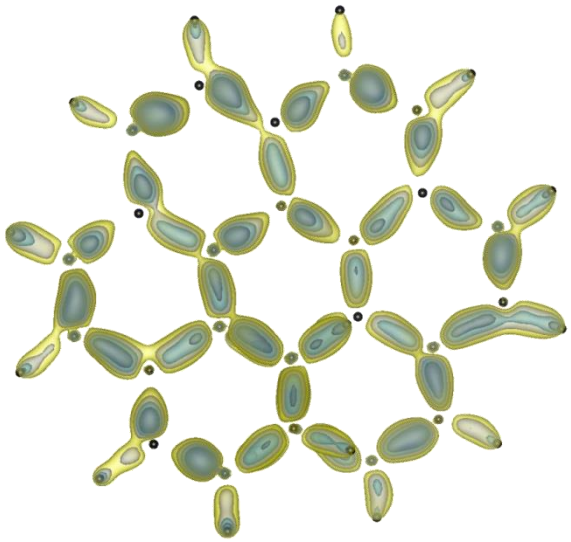
- Enzymatic optical sensor and optical fiber biosensor of glucose
- Printed optical chemical sensors
- Development of new analytical methods
- Analytical services to the research departments of ICPF
- Highly efficient catalyst and process for degradation of resistant antibiotics
- Macroporous titanium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

Research projects

Electron density distribution in polycyclic aromatic compounds through experiments; liquid state vs. solid state

(J. Sýkora, sykora@icpf.cas.cz; joint project with Charles University and Institute of Physics of the CAS; supported by GACR, project No. 15-12719S)

Project combines two experimental procedures to gain information about the bonding environment focusing on polycyclic aromatic compounds. The indirect spin-spin coupling constants $^{n}J(^{13}C\text{-}^{13}C)$ will be measured by means of advanced NMR spectroscopy. The ^{n}J values reflect the electron density distribution between two particular atoms. The NMR data will be correlated to the structural parameters (bonding distances and angles) provided by X-ray single crystal analysis. The found correlations will enable mutual prediction of these data. Both data types will also serve for the calibration of DFT calculations. Furthermore, suitable single crystals will be selected for experimental determination of charge density distribution. The results (critical points, partial charges etc.) will be also correlated to the original NMR data and also compared to DFT results. Final analysis of the liquid state (NMR) and vacuum (DFT) data when compared to XRD data will reveal the contribution of the intermolecular interactions in the packing to the final electron density distribution in a given molecule.



X-ray charge density analysis of [6]helicene

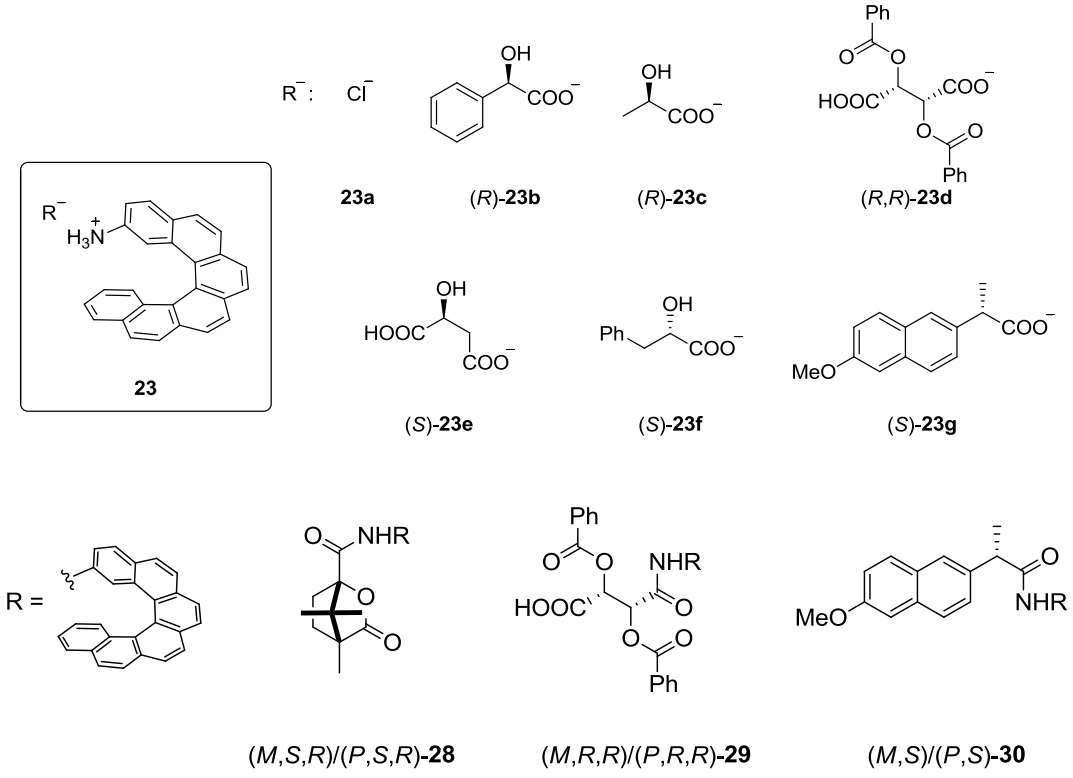
Chiral separation of helicenes

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

In the quest of our previsou activities we have turned our attention to preparation of diastereomeric salts and amides derived from 2-amino[6]helicene as an important intermediate in further synthesis (Scheme below). It was found that diastereomeric salts are not sufficient for chiral separation since the stereocenter is too far from inherently chiral helicene backbone. Thetrefore we have focused on preparation of amides starting from chiral carboxylic acids. All chiral amides exhibited strong interactions in NMR spectra, however only aromatic ones can be separated on standard silicagel stationary phase with diastereomeric excess exceeding 90%. Optimization of the procedures is currently ongoing.

Electronically deficient cinchonidine and fluorenone CT-agents for complexation of unsubstituted helicenes prepared in prevous year were thoroughly studied by means of NMR.

Results obtained will be further used for improvement of structures in order to improve enantiodiscrimination abilities and increase stability constant.



Diastereomeric salts and amides derived from 2-amino[6]helicene

Synthesis and Characterization of a Helicene-Based Imidazolium Salt and Its Application in Organic Molecular Electronics

(J. Storch, storchj@icpf.cas.cz; project supported by ICPF)

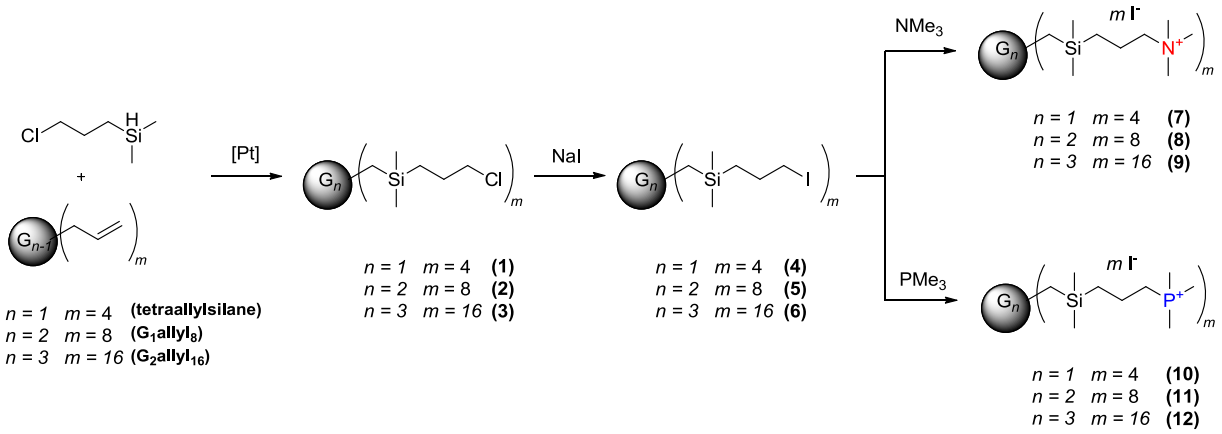
This work is focused on preparation of substituted imidazolium cation by [6]helicene backbone in order to improve helicene properties for the surface immobilization and enhancing the solubility in polar solvents. The deposited layer was used for the development of organic molecular semiconductor device and construction of novel type of fully reversible humidity sensor. [Ref. 28]

Helicene-Imidazolium salt spincoated on SiO_2 substrate with annealed gold contacts and the SEM micrographs of the amorphous (bottom) and the crystalline (upper) thin film after thermal treatment at 100 °C

Novel carbosilane dendrimers for biomedical applications - interactions with biomolecules and biomembranes

(T. Strašák, strasak@icpf.cas.cz; supported by GACR, project No. 15-05903S)

We designed and synthesized novel types of generation 1-3 carbosilane dendrimers (CS-DMMs) surface modified with various types of phosphonium and ammonium terminated CS-DDMs. In the first step carbosilane dendrimers with chloropropyl terminal were synthetized via hydrosilylation of allyls terminated starting compounds by (3-chloropropyl)dimethyl-silane. Chloropropyl functionality was subsequently transformed to iodopropyl by Finkelstein reaction. Ammonium and phosphonium groups were connected by quarterisation of trimethyl amine or an appropriate phosphine by iodopropyl-terminated dendrimers. Publication is in preparation.

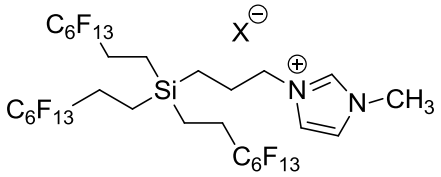


Synthetic routes leading to cationic carbosilane dendrimers

Highly fluorous cyclopentadienes for applications in catalysis

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

Fluorous ionic liquids based on 1-methylimidazolium substituted in position 3 with 3-[tris(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)-silyl]propyl group were synthesized as precursors of fluorous N-heterocyclic carbenes functioning as catalysts of redox esterification of α,β-unsaturated aldehydes. The reaction runs smoothly with primary and secondary alcohols and aldehydes that do not have a strong electron donating group. A model reaction was used to measure reaction kinetics with the salts and with a non-fluorous precatalyst $[BMIM]^+I^-$. The reaction was also tested with supercritical CO_2 as the solvent. [Refs. 29, 35]



(5a) X = I
(5b) X = BF_4
(5c) X = PF_6
(5d) X = Br

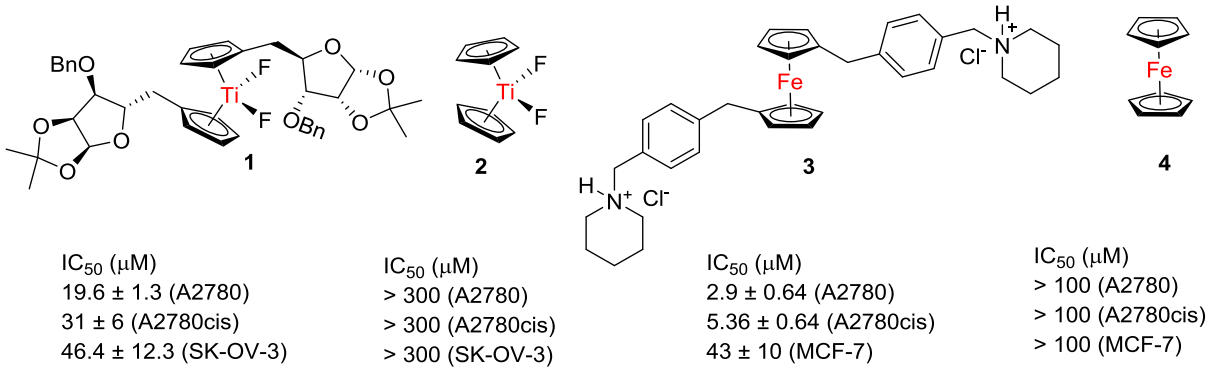
Fluorus ionic liquids

Antitumor properties and mechanism of action of metallocenes modified by carbohydrate or heterocyclic substituents

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

The accidental discovery of cytotoxic properties of cisplatin [*cis*-Pt$(NH_3)_2Cl_2$] in 1965 initiated a continuous interest in anti-cancer properties of other transition metal complexes. Metallocenes and metallocene dihalides and pseudodihalides were soon identified as promising anti-cancer drug candidates. Titanocenes and ferrocenes were among the first metallocenes reported for anti-cancer properties. The cytotoxic activity, solubility, hydrolytic stability and other medicinally relevant properties of metallocenes are substantially influenced by substituents attached to the cyclopentadienyl ring. We initiated a synthetic and biomedical program focused on titanocenes and ferrocenes modified by a carbohydrate or heterocyclic substituents at the cyclopentadinyl ring. Titanocene difluoride substituted by *O*-protected α-D-ribofuranos-5-yl moiety **1** exhibited higher cytotoxicity than cisplatin in A2780cis (IC_{50} 31 μM) and SK-OV-3 (IC_{50} 46.4 μM) human ovarian cancer cell lines (values for cisplatin: IC_{50} 50 μM and 175 μM, respectively) [Ref. 13]. Unmodified parent titanocene difluoride **2** was inactive. Further studies suggested that a stress of the endoplasmic reticulum followed by autophagy was responsible for the cytotoxicity of **1** [Ref. 13].

We have also prepared piperidinium-substituted ferrocene **3** [Ref. 1]. This compound showed cytotoxicity in a low micromolar range in human ovarian A2780 (IC_{50} 2.9 μM) and A2780cis (IC_{50} 5.36 μM) cancer cell lines. We have also developed a simple and inexpensive electrochemical method based on differential pulse voltammetry for the determination of the uptake of **3** by cancer cells [1]. Parent ferrocene **4** showed no cytotoxic properties in the tested cell lines. This correlates with the fact that only a negligible amount of ferrocene **4** penetrated into cells as showed by our electrochemical method [Ref. 1].

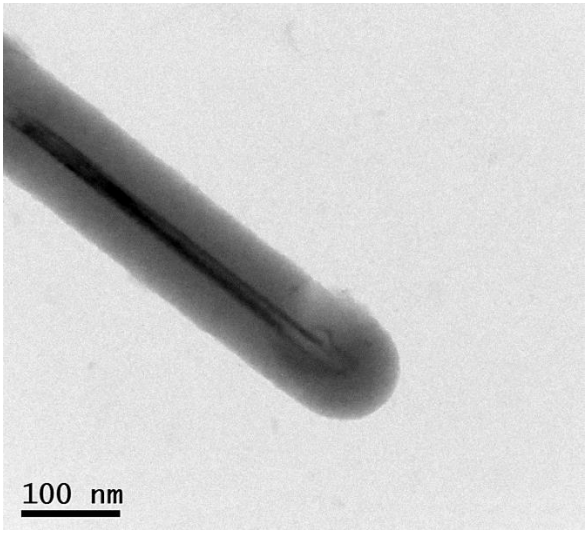


Comparison of the cytotoxic activity of modified titanocenes and ferrocenes with the parent complexes

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]

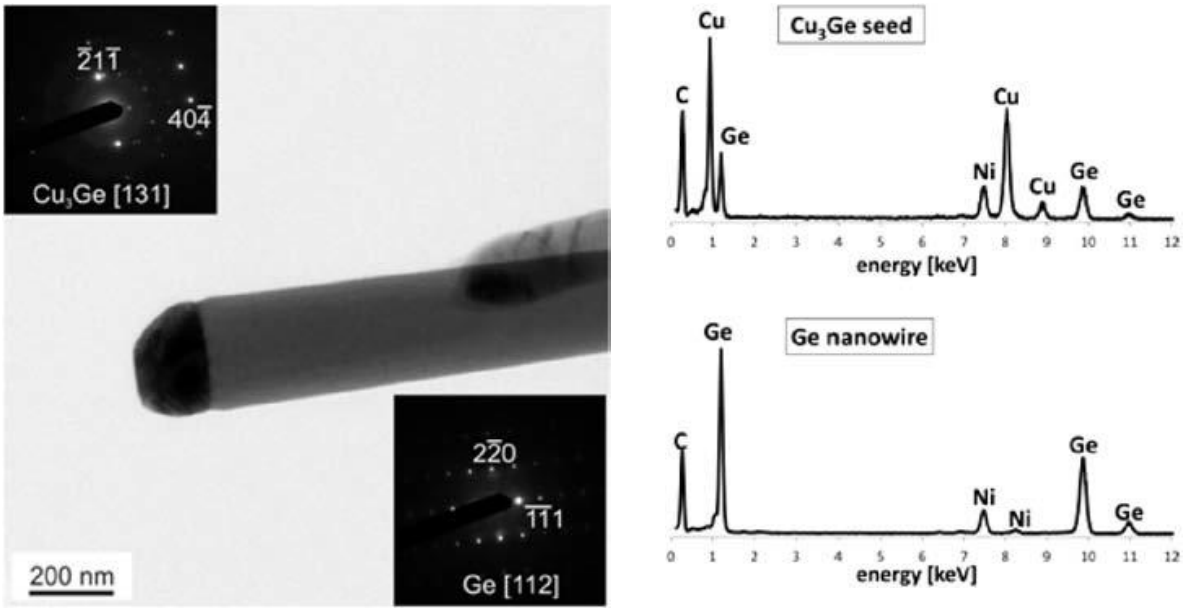


A silicon nanowire with distinguished crystalline core and amorphous jacket

Formation of $Cu_{1-x}Ge_x$ Nanoplatelets Using LPCVD of Ge_2Me_6 or Ge_2Me_6/Et_4Pb Mixture

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

Unlike synthesis of nanowires (1D nanoobjects), the synthesis of nanoplatelets (2D nano-objects) has not been performed frequently. Here we prepared Cu-Ge based nanoplatelets with a high surface-to-volume ration using low pressure CVD of Ge_2Me_6 and a mixture of $Ge_2Me_6/PbEt_4$. Nanostructured deposits are composed of $Cu_{1-x}Ge_x$ nanoplatelets, Ge nanowires and Ge nanoparticles. The nanoplatelets, which have the lateral size up to several tens of micrometers and thickness of 100-400 nm, belong to the cubic α phase of $Cu_{91}Ge_9$ alloy (Ge admixture in cubic Cu) and hexagonal ζ phase of $Cu_{85}Ge_{15}$ alloy. Nanowires composed of cubic Ge have a diameter of about 30 nm and length of several tens of micrometers. [Ref. 6]



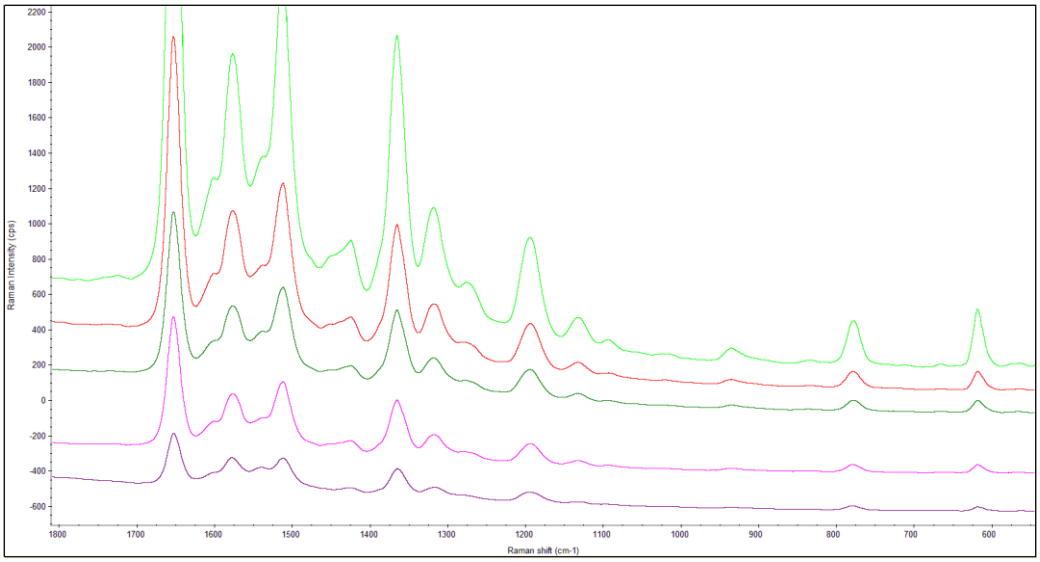
TEM observations of a deposit prepared from Ge_2Me_6: (left) bright-field image of a Ge nanowire capped by a Cu_3Ge seed and (right) EDX spectra of nanowire and the seed

Novel sensors based on laser ablated graphene

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

Research was focused on optimization of SERS properties of graphene based substrates and demonstration of their ability to enhance Raman scattering. To achieve lower detection limits of the technique, it is necessasry to tune SERS substrates by tuning metal nanoparticle plasmons to be efficiently excited. Deposition of Au/Ag alloy nanoparticles was carried out under 10 Pa of helium used as a background gas for 6 min at 60 mJ/pulse and 10 Hz laser repetition frequency. Bulk Au/Ag alloys prepared by alloying of elemental metals were used as targets. Compositions 60Ag/40Au, 40Ag/60Au, pure Au and Ag were used for deposition of corresponding metal nonoparticles. Ablation conditions were chosen to avoid graphitization of deposited graphene/polymer composites. Prepared substrates were tested for their SERS activity towards Rhodamine 6G used as a model compound. Previous study revealed this compound as the most active model for our SERS system including Raman spectrometer with 473 nm excitation line.

Rh6G was prepared as a solution (effective concentrations 10^{-5} - 10^{-10}mol/l) in deionized water. Based on UV-VIS absorption spectrum, Rh6G electronic transition is centered at 530 nm, thus the SERS measurement should be regarded as non-resonant. Typical Raman spectra of the model compound obtained from Rh6G/Ag nanoparticles are shown bellow:



Rh6G/Ag SERS spectra (concentrations 10^{-6}, 10^{-7}, 10^{-8}, 10^{-9}, 10^{-10} mol/l from top to bottom)

Pure silver nanoparticles (and alloys 60Ag/40Au nanoparticles) show the best SERS properties. Increasing content of gold deteriorates the quality of spectra and gain factors of the metal nanoparticles. Our experiments demonstrate that highly non-equilibrium ablation conditions lead to homogeneous composition of Ag/Au nanoparticles and show extreme sensitivity of the SERS technique to metal surface composition.

Highly efficient catalyst and process for degradation of resistent antibiotics

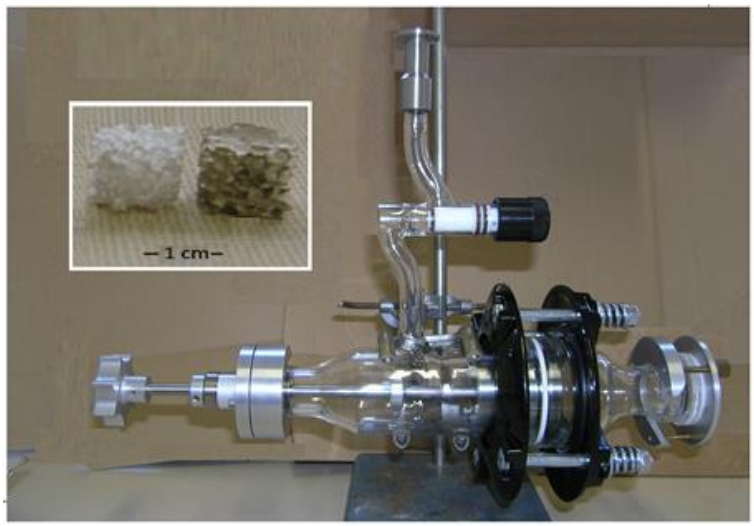
(J. Pola, pola@icpf.cas.cz; supported by TACR, project No. TA04020860)

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 ceramic carriers and will have high priorities in efficient adsorption of pollutant molecules to high-surface mesoporous structure and in pollutants degradation taking place exclusively on the incorporated grains.

In 2015, ferrous spinels (magnetite, ulvospinel, chromite, hercynite), synthesized and available as raw materials served as bulk precursors for UV and IR laser ablative deposition of films on flat Ta and porous alumina surfaces. These films were examined by electron microscopy in order to determine stability of these spinels in the laser plume and their modification in the laser ablative process. Functional samples of porous catalysts to be used in Fenton degradation of antibiotics in waste water have been prepared by laser ablative deposition of magnetite, one of the studied ferrous spinels, on porous substrates from alumina and lupek by the use of pulsed radiation from TEA CO_2 a Nd:YAG lasers.

The samples were characterized by mercury porosimetry and by means of SEM and BET analyses. They possess sufficient mechanical stability suitable for the use in filtration beds of flow reactors.



Set-up for laser ablative deposition of spinels on porous alumina substrates

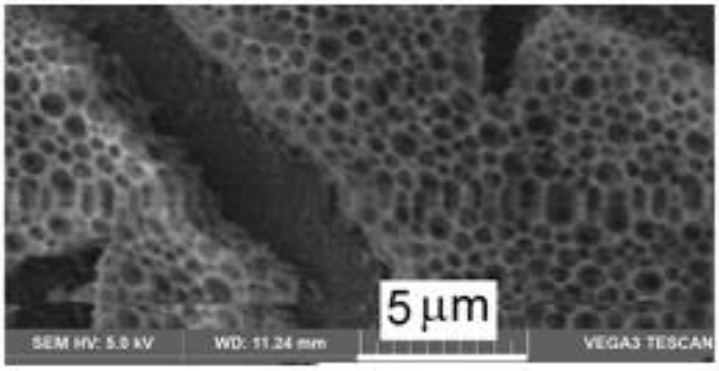
Porous and macroporous titanium surfaces with embedded submicrometer-sized Si-, SiO_x- and TiO_x- moieties for enhancing bone osseointegration and adhesion to titanium implants

(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.

In 2015, an examination of the sol-gel polymerizing TiO_2 and SiO_2 progenitors for producing bicontinuous titanosilicate structures, as well as micron-sized poly/metacrylate-styrene/ template copolymers-assisted polymerization of these precursors have been studied. These

polymerizations have been performed in sub-milimeter-sized porous Ti substrates and the porous silica/titania fillings have been examined by SEM analysis.



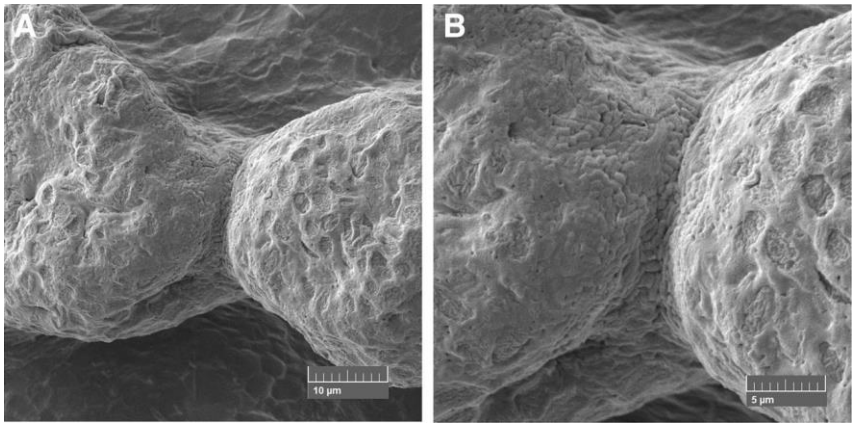
Micron-porous silica/titania filling

Printed Optical Chemical Sensors (POS)

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

Non-invasive detection of spoiled food inside a package enable the optical biosensor of biogenic amines with optical oxygen transducer. To estimate the behaviour of the sensor in parametric space, a mathematical model of the reaction–transport processes inside the sensing layer was developed. The model revealed the qualitative relations between the sensor analytical features, the characteristics of the sensitive layer and concentrations of substrates. The results of the mathematical modelling may serve as guidelines in the design of optodes for specific applications [Ref. 15].

The studies [Ref. 23, 24] demonstrate bioluminescent bioreporters *E. coli* ARL1 as a detector of contamination of bioavailable mercury in salty waters and tap water. The developed analytical assays overcome drawbacks of mercury detection with *E. coli* ARL1 via addition of tryptone into induction solution and preconcentration of mercury on the sorbent comprising yeast wall envelopes. The new detection assay with *E. coli* ARL1 made possible the detection of 0.57 µg/L of $HgCl_2$ in double-diluted artificial sea water. In tap water was detected semiquantitatively 0.025 µg/L by the induction of bioluminiscence of *E. coli* ARL1 in medium with tryptone after preconcentration using a method of standard addition. The detected mercury concentrations were below limits allowed for drinking water 2 µg/L in USA, and 1 µg/L in EU.



***E. coli* ARL1 on the sorbent with adsorbed Hg^{2+} under condition of bioluminescence induction**

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: Fluorous organocatalysis

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

Institut de Physique et Chimie des Matériaux de Strasbourg, France (CNRS): Complexation study of chiral helicene derivatives with DNA

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

Publications

Original papers

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Main fields of research

- Advanced processes for Waste-to-Energy (WtE)
- Advanced processes for gasification, gas cleaning and hydrogen production
- Urban mining
- Persistent organic pollutants and heavy metals emissions and behavior
- Environmental organic chemistry and microwave photochemistry

Applied research

- Development of a pilot plant for monitoring of Hg emissions reduction
- Design optimization of multi-stage biomass gasifier generating gas with low tar content
- Fluidized bed combustion of coal, biomass and sewage sludge
- 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

Research projects

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)

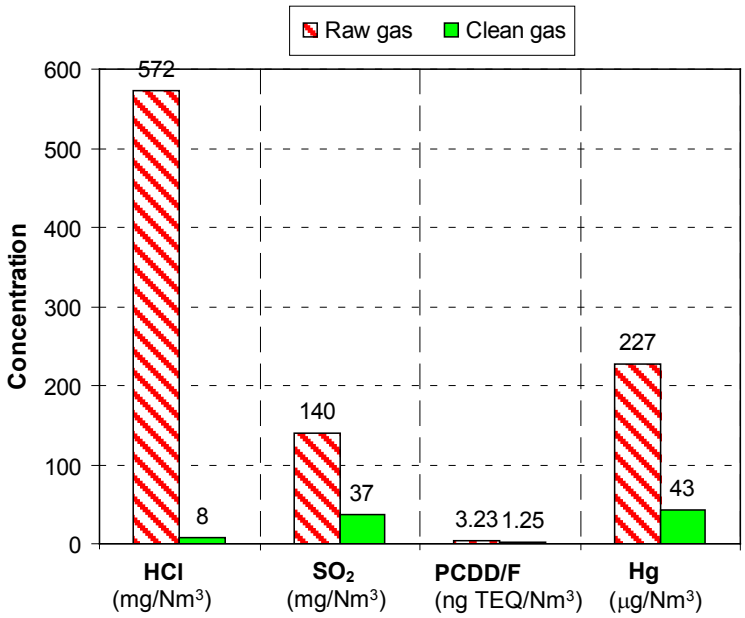
Waste-to-Energy (WtE) Competence Centre activities are aimed at increasing the competitiveness of the Czech Republic in the field of WtE. The activities are specified in such a way to be able to cover WtE from a primary idea to final products based on recent results of strategic planning, selection and 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 the leader of a work package focused on innovation and re-design of components of WtE with respect to overall energy optimization and increase of efficiency.

Our research tasks can be summarized as follows: [Refs. 4, 8-11]

- Development of new efficient dry cleaning methods for simultaneous removal of acid gases, particulate matter, NO_x, PCDD/F, and heavy metals including Hg.
- MSWI solid residues (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 thermal treatment with phosphorous recovery.

New efficient dry cleaning methods for simultaneous removal of flue gas pollutants (HCl, dust, NO_x, PCDD/F, Hg, etc.) from waste-to-energy process are studied and developed within the project. A unique apparatus for bag filters testing and optimization of dry cleaning process operating conditions was built and the effect of operational conditions on removal efficiency of each pollutant was studied. Research efforts are also focused on the development of mineral sorbents with and without chemical impregnation for dry sorption of mercury and $HgCl_2$ vapors in the temperature range 130-280 °C.



Removal of HCl, SO_2, Hg and PCDD/F by $Ca(OH)_2$-based sorbent with large specific surface, type Sorbacal® (Sindram and Walter, 2006) at temperatures 160-170 °C

Bottom ash from waste-to-energy plants contains valuable components, especially ferrous and non-ferrous metals, which can be recovered as secondary materials. The development of technology for recovering of metals from bottom ash is next task of the project. The first part of our work was the analysis of bottom ash from Czech waste-to-energy plants. We found that bottom ash contained 1.3-2.4 wt. % of non-ferrous metals, up to 10 wt. % of ferrous scrap, and 10-24 wt. % of glass. The exact distribution of valuable materials with respect to particle size was also determined. This knowledge is essential for development of an efficient recovery method.

Valuable components in MSWI bottom ash

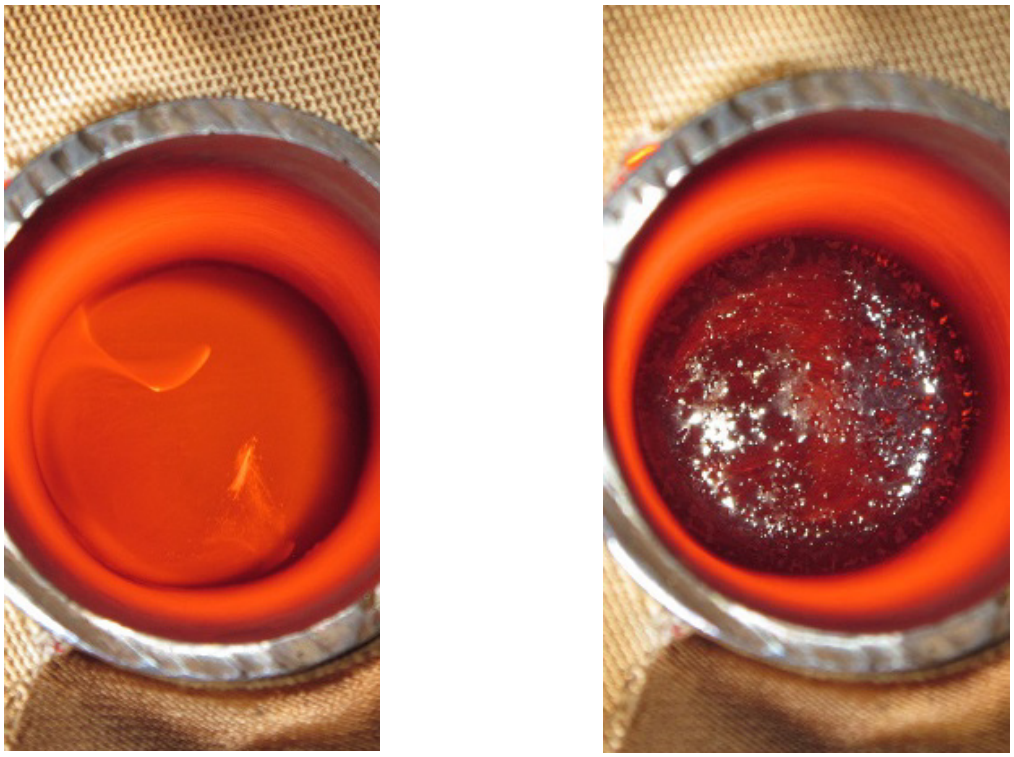
Sewage sludge incineration with subsequent phosphorus recovery from ash is the last research task of the project. We focus on finding of the optimal incineration conditions and application of primary measures in fluidized bed for minimization of gaseous pollutants. The effect of sewage sludge composition and incineration conditions on sewage sludge ash composition is also studied because ash has similar content of phosphorus like apatite (5-25 % P_2O_5) and serves as the most important secondary source of phosphorus. The development of suitable methods for phosphorus recovery from the ash is the project sub-task. Thermochemical treatment and various hydrometallurgical methods are studied and evaluated with respect to main aim of the task, which is separation of phosphorus and heavy metals and increase of phosphorus bioavailability.

Sewage sludge pellets after thermochemical treatment

Processing of radioactively contaminated ion exchangers by oxidation in molten salts

(M. Šyc, M. Pohořelý, syc@icpf.cas.cz; joint project with Research Centre Rez and CHEMCOMEX Praha, a.s.; supported by TACR, project No. TA04021660)

The project focuses on development of efficient method for thermal destruction of radioactively contaminated ion exchangers in molten salts. Various mixtures of molten salts are tested (e.g. selected carbonates or borates concentrates produced in cleaning station of the primary circuit of VVER type nuclear power plants. Main target of the project is to propose optimal conditions of process considering technological, operational, and economic factors and to verify them on the semi-pilot plant.



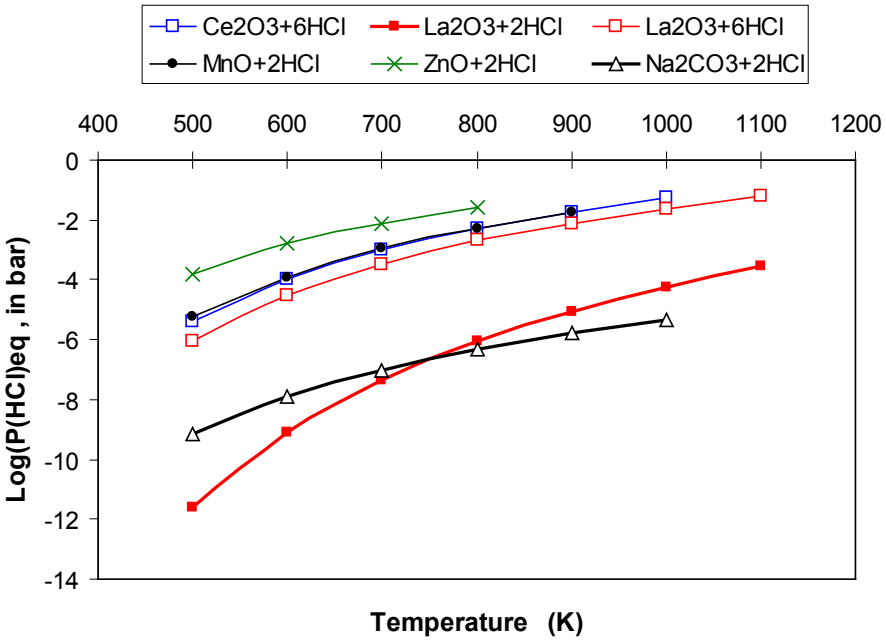
Oxidation of ion exchanger in molten mixture of sodium, lithium and potassium carbonates, on the left - volatiles incineration above the molten salts, on the right - ash layer on the top of molten salt

Cleaning of syngas 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 ^{o}C. A soda-based sorbents 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, CeO_x and $La_2O_3/La_2O_2CO_3$ serve for removal of H_2S, COS, destruction/removal of thiophene and for study of interferences (CO_2, H_2O(g) and HCl). 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 are developed and solved. Possibilities of regeneration of the sulfur compounds sorbents are assessed. [Ref. 1]



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

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).

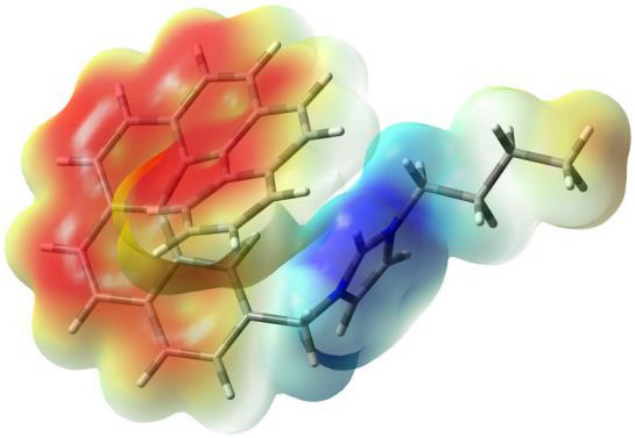
The effects of operating conditions and selective catalytic reduction on Hg concentration in flue gas will be investigated on a developed pilot plant. The result of the project solution will serve as basis for technical documentation for the existing energy sources modifications, or preliminary documentation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

Aplication in Organic Molecular Electronics

(V. Církva, cirkva@icpf.cas.cz; joint project with Palacky University, University of Pardubice, UCT Prague, Institute of Physics of the CAS, Czech University of Life Sciences Prague, Institute of Organic Chemistry and Biochemistry of the CAS, Charles University Prague, supported by MIT, project No. FR-TI3/628; TACR, project No. TA04010082 and TA01010646)

During the past 30 years, the study of organic electronics based on π-electron network molecules has made rapid progress and practical organic devices are currently being produced. Polycyclic aromatic hydrocarbons with their extended two-dimensional (2D) π-conjugated frameworks are of particular interest for this purpose as they can provide charge-transporting pathways when arranged into appropriated superstructures in the solid state.

The study was focused on the substitution of the imidazolium cation with [6]helicene to improve surface immobilization and to enhance its solubility in polar solvents. The deposited layers were used for the development of organic molecular semiconductor devices and the construction of fully reversible humidity sensor. [Refs. 2, 3, 6, 7]



Electron density isosurface mapped with electrostatic potential surface of 1-butyl-3-(2-methyl[6]helicenyl)-imidazolium bromide in the range from 0.06 (red) to 0.20 (blue)

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 a compact technology for high efficiency dry refining flue gas technology for small and mobile incinerators was developed. This refining technology 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 no sustainable water management options are available.

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 28% and for modern engines to an efficiency of 32%. On the basis of the above equipment four thermal power stations are operated in the Czech Republic, one facility in Slovakia and one facility is under construction in Czech Republic.

Combined heat and power generation plant in Kozumín – under construction

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

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

Project is developing 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)

The 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 lead 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 will be a technical-economical study which will 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, a part of the output will 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.

In-situ thermal desorption with use of microwaves

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.

High effective machine FT3 for pothole road repairs (http://www.iwme.cz/produkt/)

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.

Microwave reactor for drying of surfactants

Recovery of lanthanides from spent NIB magnets

(V. Gruber, gruber@icpf.cas.cz; supported by TA CR, research project Gama, project No TG01010097)

The research was focused on a chemical recovery of neodymium and other lanthanides from spent neodymium-iron-boron permanent magnets. To improve magnetic properties, NIB magnets were often doped with other elements (Pr, Dy, Co) and their composition varies. For a complete recovery of all valuable components, the two-steps isolation process was designed. First, neodymium and praseodymium have been separated from ferrous metals by fractional crystallization of complex sulfate salts. Then solvent extraction of dysprosium by bis-(2-ethylhexyl)phosphoric acid was employed. Pure neodymium, didymium and dysprosium oxides were finally obtained by precipitation of oxalates and their thermic decomposition.

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 gasification of biomass, urban mining
CIEMAT Madrid, Spain: gas cleaning, processes for carbon capture and storage (CCS)
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

Visits abroad

M. Jeremiáš, Cranfield University, United Kingdom

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Biorefinery research centre of competence (BIORAF)

BIORAF
Centrum kompetence pro výzkum biorafinací

(O. Šolcová, solcova@icpf.cas.cz; joint project with Institute of Chemistry and 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.; supported by TACR, project No. TE01020080), project web pages (http://bioraf.cz/).

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*.

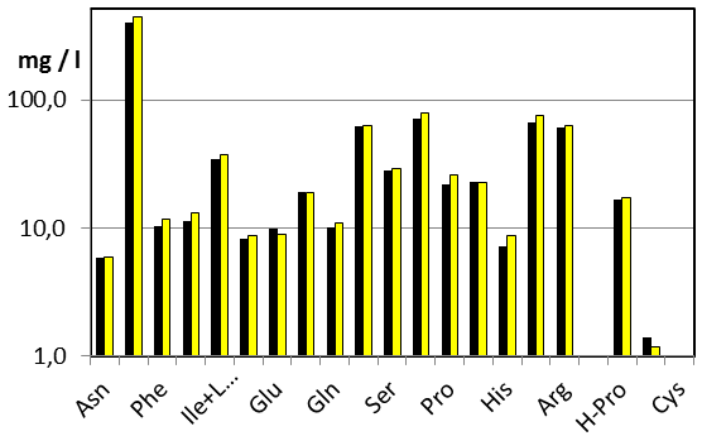
The project brought awareness into society about the biorefinery area as new scientific direction, that in Czech Republic was virtually absent before creation of BIORAF, but has big perspective for development of small and medium size companies.

Pressure hydrolysis of protein in waste of chicken cartilage and feathers in the presence of carbon dioxide

(J. Hanika, O. Šolcová)

Proteins hydrolysis of chicken cartilage and feathers were carried out at increased temperature (till 120 °C) and in the presence of carbon dioxide (partial pressure 10-20 bar), which dissociates in water solution forming an acidic environment supporting the reaction. Carbon dioxide was easily detachable from the reaction mixture at the end of process. Bench scale tests were performed using a mixed autoclave (volume 2.5 L, mixing time 5 h). The resulting aqueous solution of amino acids contained in the same representation as peptides forming collagen and keratin of raw material. The reaction conversion was proportional to carbon dioxide partial pressure.

Pure hydrolysate



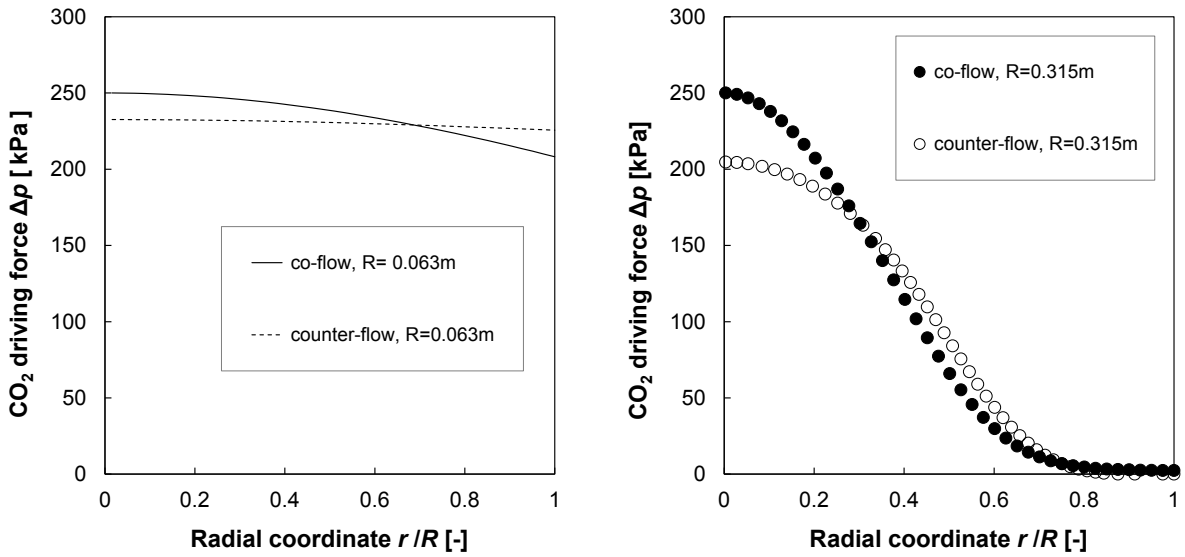
Amino acids distribution in hydrolysate mg/L

The hydrolysis product is perspective one for various applications, first, for dampening the composted agricultural waste, next could be useful as nutritional additives to livestock feed and finally as a nutrient supporting growing algae for biotechnology applications. For any culture, or nutritional usage of hydrolyzate as ingredient in feed mixtures have to be necessary to perform additional relevant field tests.

Membrane separation for biogas purification

(L. Morávková, M. Kárászová, Z. Sedláková, M. Šimčík, J. Vejražka, P. Izák)

Membrane separations were found to be a useful tool for the biogas upgrading. One of the recent break-through in biogas membrane upgrading is application of water-swollen membranes. Its big advantage consists in fact that water present in the raw biogas helps separation and thus, pre-treatment of a feed stream is not necessary such as in the other membrane separation processes. Selection of the suitable membrane material was found to be a complex procedure that includes not only separation properties but also the basic membrane characteristics. To decrease time necessary for the membrane testing before suggestion of a scale-up, determination of the mass transfer coefficients of main compounds contained in raw biogas such are carbon dioxide and methane was suggested. The mass transfer coefficients were evaluated from experiments done on two membranes supplied by Koch and Toray membrane using simple engineering procedure. Further, prediction from the model was compared to the experimental data. The missing data could be predicted using the theoretical mass transfer coefficients. However, it was found that the coupling effect has to be included in the future prediction models to obtain more precise prediction.



Koch membrane. Scale up from R = 0.063 m (experimental cell - lines) to R = 0.315 m (virtual larger cell - marks). Radial profiles of CO_2 mass transfer driving force (the difference of CO_2 partial pressures between both sides of the membrane representing the driving force). Co-flow vs. counter-flow arrangement

Microalgae for bioenergy; key technology nodes

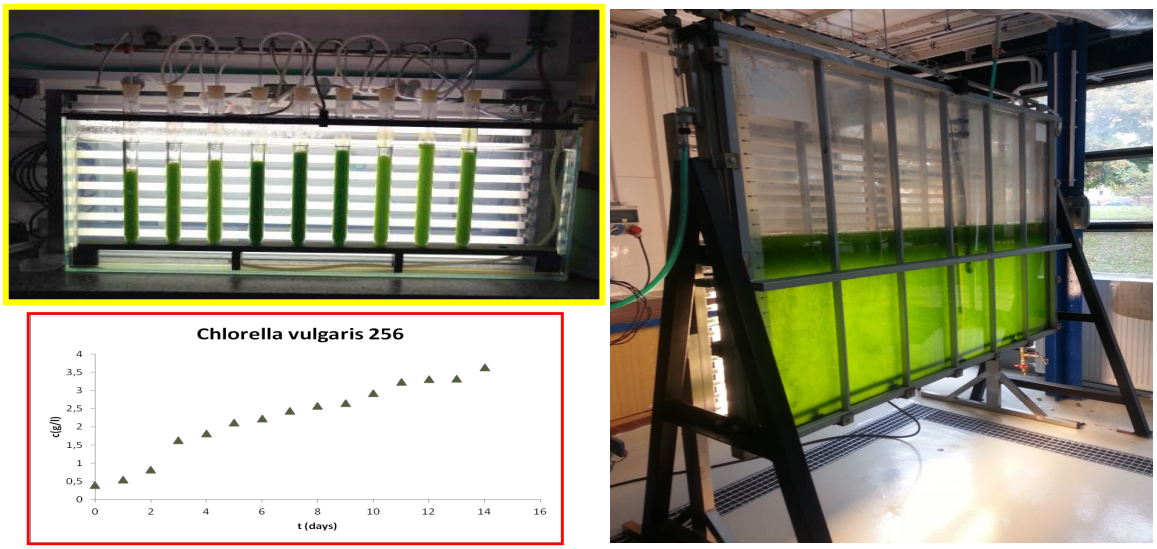
(Y. Maléterová, F. Kaštánek, M. Rousková, M. Matějková, O. Šolcová)

The three key steps, flocculation, water recycling and extraction of microalgal treatment for lipid production have been suggested and evaluated with respect to the possible environmental impacts and production costs. To avoid the energy consuming drying step the completely wet way treatment has been applied. It was verified that ammonium hydroxide can serve as the efficient and the low cost flocculation agent. The optimal flocculation conditions

were determined at pH 9. Moreover the application of ammonium hydroxide brings into the algal water solution only the biogenic elements and thus enables the water recycling for the recurring microalgae growth. Water recycling was verified for the use of 50 and 80 % recycled water.

It was confirmed that extraction of the wet microalgae can be applied instead of the dry microalgal extraction, which enables to release the energy consuming drying step. The efficiency of hexane/ethanol extraction system was found as comparable with chloroform/ methanol system; the comparative method. Moreover, not only the amount of the extraction fraction of the total lipids, but also the profiles of fatty acids was the same. Except of the relatively high extraction capacity, hexane/ethanol extraction system possesses the low volatility and toxicity for humans as well environment and mainly the low cost.

The wet way processing of the harvested microalgae for biodiesel production seems to be the low cost promising biotechnological application with the minimal environmental impact.



Cultivation set-up; growth curve of *Chlorella vulgaris*

Waxes and lipids extraction from miscanthus × giganteus stems

(M. Rouskova, O. Solcova, J. Hanika)

Plantations for experimental production of Miscanthus × giganteus and Miscanthus sinensis have been founded by the project partner AGRA Co. Tall stems of this plant contain a broad spectrum of various substances (waxes, lipids, carotenoids, etc.) being potentially exploitable in cosmetics. Extraction processing of crushed dry stems using non-polar solvent is a promising way for separation of these substances into an extract, whereas the waste raffinate containing waste biomass has, after being pressed into the form of pellets, the potential for energetic utilization as “green fuel”.

Miscanthus sinensis **Miscanthus giganteus**

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17TH E. HÁLA LECTURE (2015)

RICHARD D. NOBLE (University of Colorado, Boulder, USA), on 16 April 2015:
"Novel Membranes for Improved Separations"

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

Annual Report 2015

Vladimír Církva (Editor)

Graphical Editing: Vladimír Církva and Zdeněk Wagner
Typesetting: Zdeněk Wagner

Published 2016
Institute of Chemical Process Fundamentals of the CAS, v. v. i.
Rozvojová 135/1
165 02 Prague
Czech Republic
www.icpf.cas.cz

Printed 2016
WOW spol. s r.o.
Washingtonova 25
110 00 Prague
Czech Republic
www.wow.cz

ISBN 978-80-86186-79-5