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

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

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General Information

The Institute of Chemical Process Fundamentals (ICPF) is one of six institutes constituting the Section of Chemical Sciences of the Academy of Sciences of the Czech Republic. 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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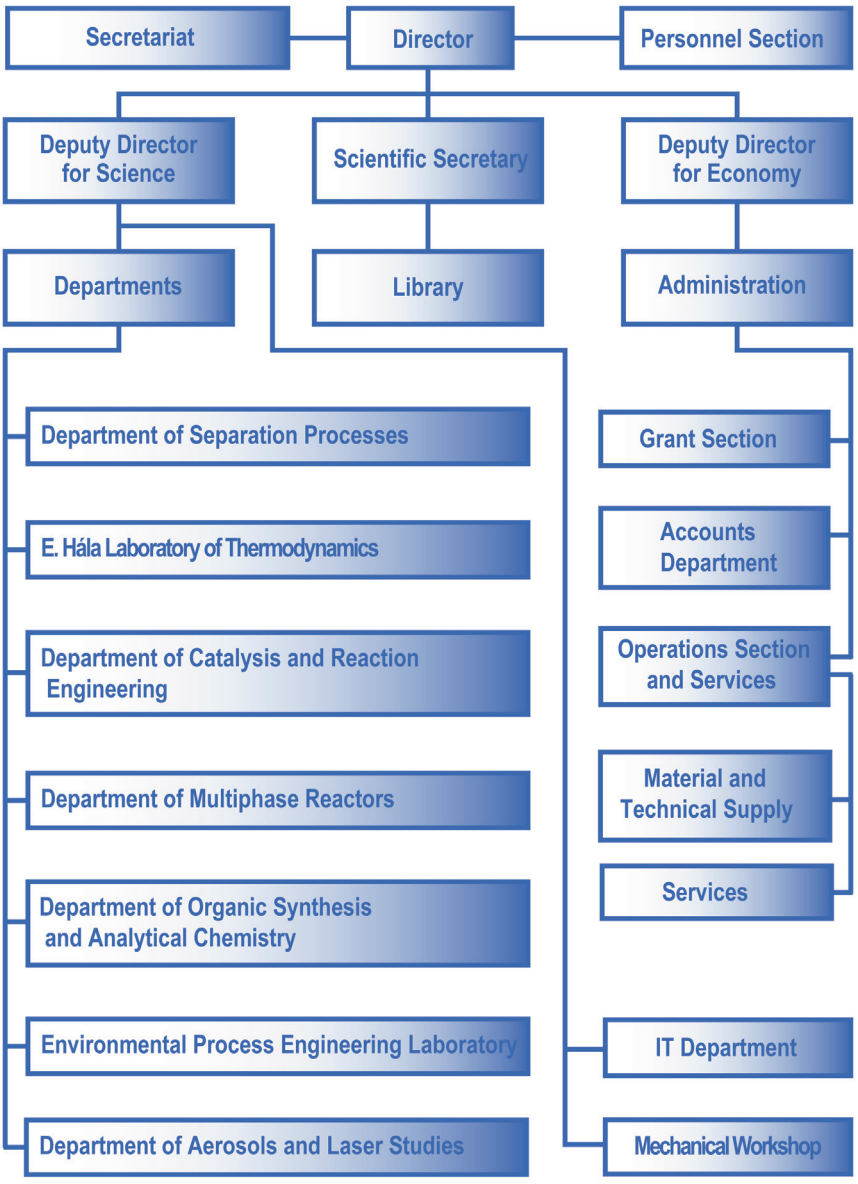
Organization Chart



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STAFF

(December 31, 2013)

Category	Number of Employees
Research	82
Research Support	69
Technical	10
Administrative	14
Services	11

BUDGET 2013

(20.20 CZK ≈ 1 US$, 27.33 CZK ≈ 1 €)

Resources	Million CZK
Institutional support based on Institutional Research Plan	77
Targeted support from Grant Agencies and R&D Programs in the Czech Republic	59
Foreign R&D Funds and European Programs	10
Contracts with industry	8
Other resources	27
Total Resources	**181**

Expenses	Million CZK
Personal expenses including mandatory insurance	95
Purchase of material	19
Purchase of services	14
Repairs and maintenance	13
Depreciation of fixed assets	16
Travel expenses	4
Energy, water, and fuels	5
Total other expenses	8
Total other expenses	**174**

Profit	Million CZK
Total	**7**

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Fields of research

- Hydrodynamics of two phase flow in micro/macro channels
- Sulfur dioxide oxidation, sulfation and sulfonation
- Kinetic studies of heterogeneously catalyzed reactions in microreactor
- Design of counter-current vibrating plate extractor (VPE)
- Fluorinated hydrocarbons as potential solvents in liquid-liquid extraction processes
- Supercritical fluid extraction of biologically active substances
- Kinetics of supercritical fluid extraction
- Chemical and enzymatic reactions in supercritical CO_2
- Mass transport in polymeric membranes, mutual influence of permeating substances
- Mass transport through ionic liquid membranes
- Membrane separation of methane and CO_2 mixtures
- Separation of racemic mixtures
- Separation of gasoline vapors from air by supported ionic liquids membranes
- Description of the flow of condensable gas through the porous medium

Applied research

- Hydrodynamics of annular gas-liquid flow
- Application of microreactors for gas phase catalytic reactions
- Liquid-liquid extraction of luminophores, recycling of Y and Eu
- Liquid-liquid and supercritical fluid extraction and refining of plant extracts
- Purification of biogas by supported liquid membrane
- Extraction of insecticides from plants

Research projects

Flexible, fast and future production processes (F^3 Factory)

(V. Jiřičný, jiricny@icpf.cas.cz; FP7 collaborative large integrated project, Theme NMP-2008-3.2-1; supported by EU under Contract No. CP-IP 228867-2 F^3 Factory)

The goals of the projects are in improvements of EU chemical industry's competitive position by development modular continuous plant (F^3 Plant) which combines world scale continuous plant efficiency, consistency and scalability with the versatility of batch operation. Based on the extensive hydrodynamic study, the microsulphonator pilot plant prototype was designed, manufactured and tested in ICPF. Together with Procter&Gamble, ICPF participated in the upgrade of the industrial pilot plant with the aim of installing the new microsulphonator reactor. During 2013 the microsulphonator was installed into Procter&Gamble pilot plant and its operation was successfully tested. The obtained product reached two our of three target quality criteria. ICPF team also tested the advanced method for the SO_2 analysis (defined in 2012) in the pilot plant installation, and participated in the pilot plant experiments with the pilot plant microreactor for sulfur dioxide catalytic heterogeneous oxidation.

Pressure drop during the annular gas-liquid flow

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

Based on the successful pilot plant tests during the F^3 Factory project, Procter&Gamble was interested in the continuation of our cooperation within the research project focused on the hydrodynamic measurements of annular gas-liquid flow. The existing experimental unit was modified to accommodate the larger reactors and the hydrodynamic experiments were carried out in the area of interest of the commercial partner. The most important evaluated parameters were pressure drop and flow regime.

Application of microreactors for gas phase catalytic reactions

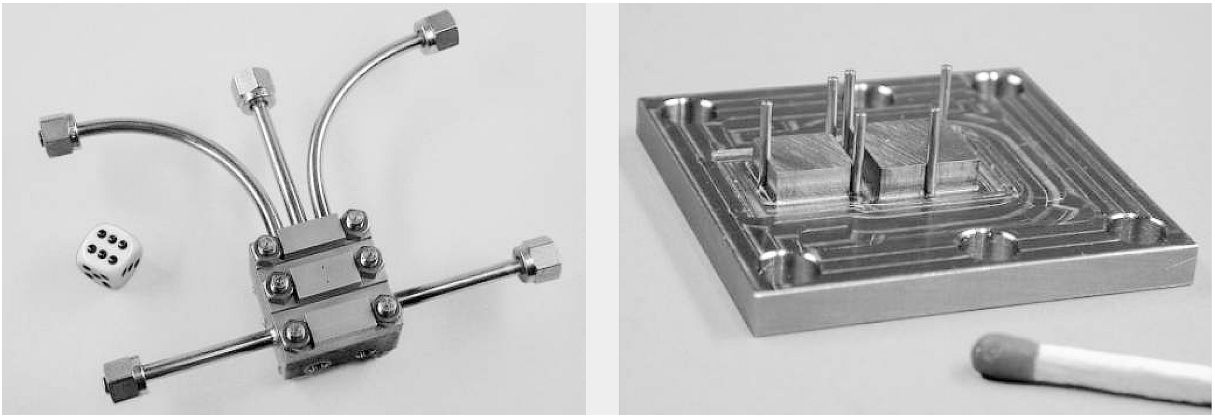
(P. Stavárek, stavarek@icpf.cas.cz; research contract with Momentive Specialty Chemicals)

The feasibility of application of microreactors was assessed and evaluated for the gas phase catalytic oxidation reaction. Based on this feasibility study, the preliminary design of an experimental laboratory apparatus was prepared.

Synthesis methylchoride in a microreactor

(Z. Vajglova, vajglova@icpf.cas.cz; study stay at Åbo Akademi University, Finland)

A reactor setup consisting of two stainless steel microreactors (Gas Phase Micro Reactor with mixer, GPMR-mix, by Microinnova Engineering GmbH, Austria) coupled in series was used for production of methyl chloride by hydrochlorination of methanol. The influence of temperature on the methanol conversion and selectivity towards methyl chloride were investigated. A maximum conversion of 97.6 % and a selectivity of 98.8 % could be reached, which is close to the calculated thermodynamic equilibrium. Comparison with results obtained from a single microreactor and a modified setup of the two microreactors revealed that the serial coupling resulted in a dead volume with a blind activity which cannot be neglected when describing the setup. Furthermore, separation of gaseous products using condensers was investigated and as well as the composition of obtained gas and liquid phase.



Gas Phase Micro Reactor (GPMR) with mixer and internal heating cooling (left)
Top housing plate of reactor with mixer and reactor stack (right)

Applications of liquid-liquid extraction in recovery of rare earth metals

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

The object of this project was to perform laboratory and pilot plant tests for recycling of luminophores from waste compact fluorescent light bulbs (CFLs). The process consists of selective extraction of valuable yttrium and europium and removal of toxic mercury. The experimental results were used as a basis for the design of the pilot plant unit with counter-current vibrating plate extractor (VPE) at cooperating University. Common patent was applied. [Ref. 20]

Pilot plant unit for recovery of luminophores

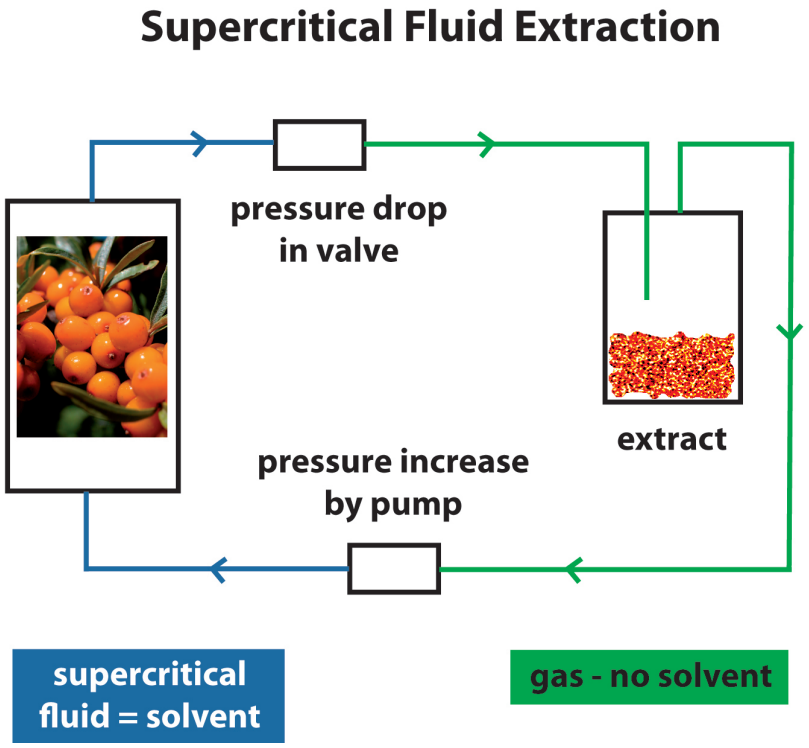
Research and development of new products for complex plant protection

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

New preparations for eco-agriculture are being developed on the basis of hydrodistillates and supercritical extracts from tropical plants with high content of the biologically active substances.

Plant material supplied from South Africa is submitted to supercritical fluid extraction, hydrodistillation and maceration in order to assess the suitability of the methods used for obtaining extracts with maximum biological activity. The supercritical fluid extraction is conducted under different experimental conditions. The insecticidal activity (antifeedancy, acute toxicity, and chronic toxicity) of isolates is measured on larvae of *Spodoptera litoralis*. Antifungal bioassay is carried out on the isolates as the inhibition effect on the growth of model pathogenic and toxinogenic fungi. The chemical composition of isolates is determined by GC/MS technique. [Refs. 11, 12]

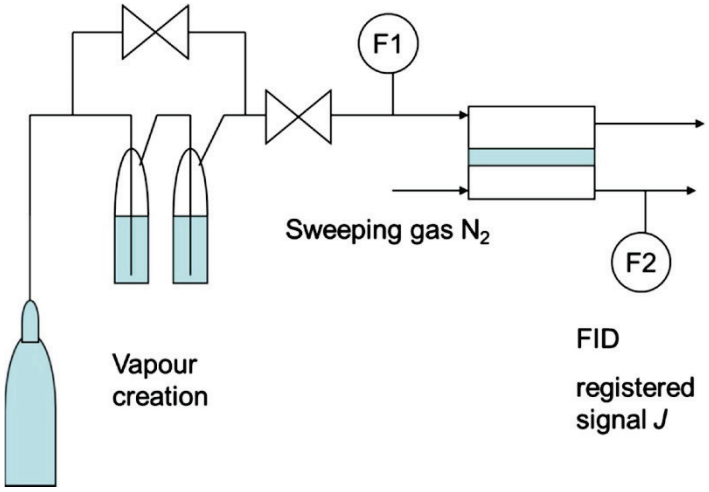
Solubility of isolated components in supercritical CO_2 is measured using the dynamic method and the extraction kinetics is simulated by phenomenological models. [Refs. 1, 8, 13]



Study of polymeric membrane swelling and make use of this effect for increasing its permeability

(P. Uchytil, uchytil@icpf.cas.cz; joint project with IMC, supported by the GACR, project No. P104/09/1165)

The location of the phase change inside membranes and swelling of the membrane material during toluene transport in a polyethylene membrane were investigated. The special experimental sweeping-gas set-up was proposed and constructed to obtain all transport parameters in polymeric membranes (flux, diffusivity and sorption). Study of an addition of a convenient substance was performed on several types of membranes that were prepared in cooperation with the foreign partner (Prof. S.-Y. Suen). On the basis of the obtained results new membrane separation process was designed and the high separation efficiency of gas separation was experimentally verified and applied for patent. [Refs. 9, 10, 21]

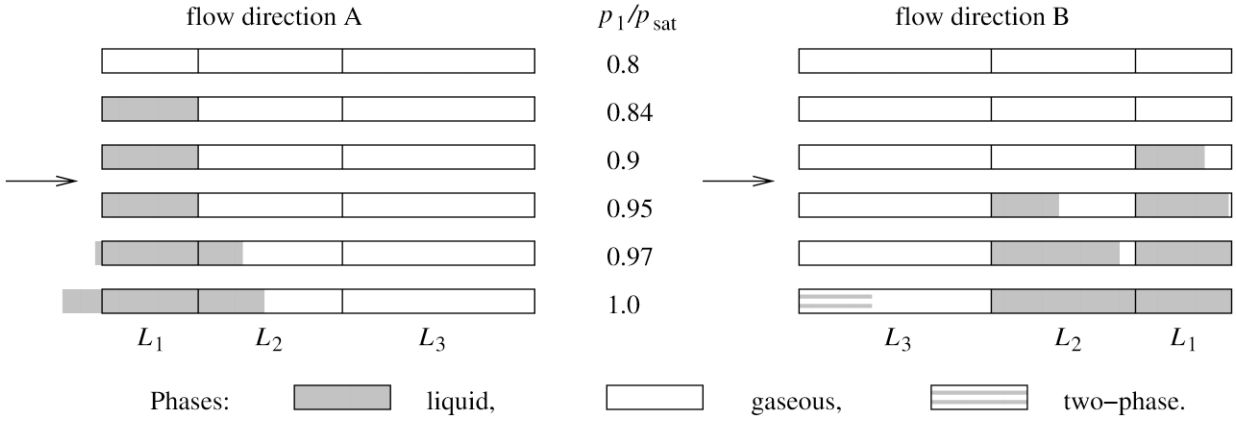


Sketch of the permeation apparatus

Flow of saturated vapors through porous membranes

(J. Řezníčková, reznickova@icpf.cas.cz; joint project with Institut für Strömungsmechanik und Wärmeübertragung Technische Universität Wien; supported by MEYS, MOBILITY, project No. 7AMB12AT010)

Mathematical model of the vapors flow through asymmetric porous membranes was developed. The flow is modeled using the energy balance and accounting for capillary condensation, for the transport of the enthalpy of vaporization, and for the temperature variation due to the Joule-Thomson effect. Transport of isobutane through an asymmetric ceramic membrane consisting of three different layers has been investigated. In the case studied, the mass flow rate can become several times larger in one flow direction than in the other flow direction. It depends on the state of vapor saturation and on the porous structure of the membrane in which direction the mass flow rate becomes larger. The large differences in the mass flow rate occur if the fluid condenses in one or in several parts of the membrane in one flow direction, but it does not condense or condenses in different parts of the membrane in the other flow direction. This finding may be generalized. For the flow of a vapor which is in a state close to saturation, the mass flow rate through an asymmetric membrane in one flow direction may differ very much from the mass flow rate in the other direction.



Phase state of the permeant in the membrane layers for both flow directions at different upstream relative vapor pressures, for $p_1 - p_2 = 0.5$ bar. Thicknesses of the individual layers are not to scale

Separation of volatile organic compounds (VOCs) from air

(P. Izák, izak@icpf.cas.cz; joint project with ICT Prague; supported by GACR, project No. P106/10/1194)

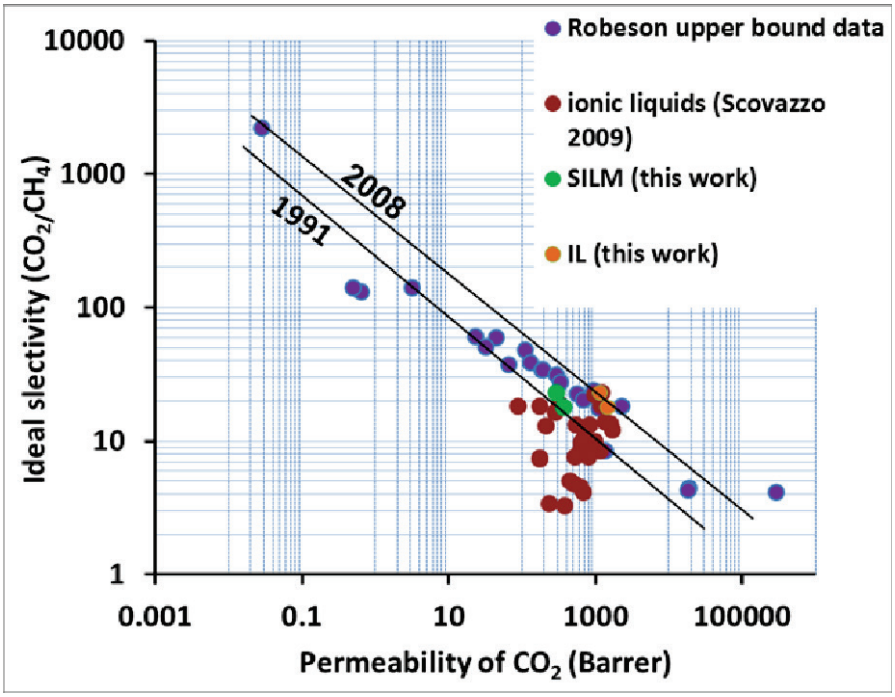
Aim of this project is a development and application of membrane techniques to increase the affectivity of classical separation processes with help of computer simulations and theoretical modeling. In most of processes the goal of separation techniques is to recycle vapor phase, which was lost in a sweeping gas.

Ionic liquid polymer gel membranes based on poly(vinylidene fluoride-co-hexafluoro-propylene) (p(VDFHFP)) were prepared by solvent casting from a solution in acetone. The membranes contain from 20 wt. % to 80 wt. % of pure or mixed ionic liquids based on the imidazolium cation: 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][TFSI]) and 1-hexadecyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide ([HdMIM][TFSI]). The gas transport through the membranes prepared in this study was evaluated in the temperature range of 20 - 60 ºC, which includes the melting point of the high temperature ionic liquid [HdMIM][TFSI]. These permeation measurements show a significant increase of the permeability in the presence of the IL mixture, especially for carbon dioxide. This suggests a potential application in gas separation membranes, for instance for natural gas treatment or for CO_2 sequestration from flue gas [5].

In addition, we present a novel method for the treatment of raw sorption kinetic data recorded by a gravimetric sorption apparatus equipped with calibrated quartz (McBain's) spiral balance. The mentioned treatment enables to eliminate overlapping mechanical oscillations of the spiral balance (caused by the initial charging of the sample gas/vapor into the evacuated measuring chamber) and to successfully reconstruct the real elongation of the spiral caused by gas/vapor sorption into a polymer material. This allows to calculate even from highly noised sorption data the accurate values of gas/vapor diffusion coefficients [2].

Molecular dynamics simulations of n-hexane adsorbed onto the interface of 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide ([bmim][Tf_2N]) are performed at three n-hexane surface densities, ranged from 0.7 to 2.3 μmol/m^2 at 300 K. For [bmim][Tf_2N] room temperature ionic liquid, we use a non-polarizable all-atom force field with the partial atomic charges based on ab initio calculations for the isolated ion pair [7].

Successful practical application of ionic liquid (IL) membranes requires good understanding of their basic transport properties and the role of the IL itself and its polymeric support. Within this work, two approaches to the calculation of mass transfer coefficients of gases in supported ionic liquid membranes were applied. The first one applies the models and data reported on diffusivity and solubility of gases in pure ionic liquids in the literature, in combination with porosity and tortuosity of the support. The second one is based on fitting of experimental data obtained from two ionic liquid membranes. The results of both approaches were compared and used to predict the properties of ionic liquid membranes. It was found that the model based on data of pure liquids overestimated the mass transfer coefficient signify-cantly. The correlation diagram known as the Robeson plot is frequently used to compare the permeability and selectivity of a new membrane with the already reported data. It combines the Robeson upper bound data with the determined results and the data of pure ionic liquids reported previously [6].



Robeson upper bound data and ionic liquid data

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

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

The goal of the proposal is to develop new membrane separation techniques for successful resolution of racemic mixtures allowing optimization of the therapeutic value of enantiomeric drugs (pharmacological and toxicological) and avoiding their adverse effects. The key objective is to separate enantiomers by a new membrane separation method, based on the proposed supported chiral room temperature ionic liquid membrane, that has never been studied yet. In comparison with classical methods employed earlier, it should show higher efficiency and cost effectiveness in the processes of enantiomer separation. New chiral hyper-branched polyimide membranes modified by end-capping with (+) or (-) – isopinocampheyl-amine were prepared and the careful characterization of the membranes by spectroscopic methods was done. Further, the results of comprehensive research on transport of particular enantiomers through hyperbranched polyimide membranes modified by end-capping with (+) or (-) – isopinocampheylamine and cellulose derivative membranes were described. Diffusion coefficients, total sorption values and separation factors for enantiomers of racemic mixtures were measured. The new pertraction cell for measurement of diffusion coefficient was used.

We developed an all-atom non-polarizable force field for simulations of two chiral room temperature ionic liquids derived from 1-n-butyl-3-methylimidazolium bromide ([bmim][Br]); namely, (*R*)-1-butyl-3-(3-hydroxy-2-methylpropyl)imidazolium bromide (hydroxypropyl) and 1-butyl-3-[(1*R*)-nonyl]imidazolium bromide. The force field adopts the CHARMM parameters for intramolecular and repulsion-dispersion interactions, and it employs reduced partial atomic charges of the ions which we derived by quantum mechanical calculations.

International co-operations

CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials
Institut für Strömungsmechanik und Wärmeübertragung Technische Universität Wien: Flow of saturated vapors through porous membranes
Institute of Chemical Engineering, Sofia, BAS: High-pressure phase equilibria
Institute of Macromolecules, St. Petersburg, RAS, Russia: Membrane separation
Institute on Membrane Technology, CNR, Italy: Novel composite membranes containing ionic liquid and selected polymers for specific gas/gas, gas/vapor and vapor/vapor separations
KIT Karlsruhe, Germany: Design of pilot plant size microreactor for sulfur dioxide catalytic heterogeneous oxidation
Momentive Specialty Chemicals, Czech Republic: Application of microreactors for gas phase catalytic reactions
National Chung Hsing University, Taiwan: Preparation of Dense Homogeneous Polymeric Membranes and Study on Their Gas Permeation Properties
Otto von Guericke University of Magdeburg, Germany, Max-Planck-Institut für Dynamikkomplexer technischer Systeme. Magdeburg: Mass transport through porous membranes
Procter&Gamble, Belgium: Research and developments of microapparatus characteristics
Procter&Gamble, Belgium: Hydrodynamics of micro reactor for sulfonation
Procter&Gamble, Belgium: Hydrodynamics of annular gas-liquid flow
Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapors through porous membranes
Technical University of Lisbon, Portugal: Supercritical extraction of biological compounds from aromatic plants
University of Colorado, Boulder, CO, USA: Mass transport during vapor permeation and pervaporation, ionic liquids
University of Burgos, Spain: Enzymatic reactions of oil in supercritical CO_2 medium
University of KwaZulu-Natal, Republic of South Africa: Liquid-liquid extraction processes with fluorinated hydrocarbons, recovery of luminophores

Visits abroad

J. Křišťál, Procter&Gamble, Belgium (3 weeks)
V. Jiřičný, Procter&Gamble, Belgium (2 weeks)
P. Stavárek, Procter&Gamble, Belgium (5 weeks)
Z. Vajglová, Åbo Akademi University, Finland (6 months)

Visitors

M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
F. Euzenat, ENSIASET Toulouse, France
A. Palavra, Technical University of Lisbon, Portugal

Teaching

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

J. Hanika: ICT, Faculty of Chemical Technology, course "Pharmaceutical Engineering"
H. Sovová: TU Darmstadt, Life Long Intensive Program "Process Intensification by High Pressure Technologies – Actual Strategies for Energy and Resources Conservation"

Publications

Original papers

[1] Bucic´-Kojic´ A., Sovová H., Planinic´ M., Tomas S.: Temperature-Dependent Kinetics of Grape Seed Phenolic Compounds Extraction: Experiment and Model. *Food Chem.* 136(3-4), 1136-1140 (2013).

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Review papers

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Books and monographs

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Chapters in books

[17] Hanika J.: Decades of German-Czech Common Research on Periodic Operation of Trickle Bed Reactors. In: *Jubiläumsband 60 Jahre Dresdner Verfahrenstechnik*, pp. 194-197, Technische Universität Dresden, Dresden 2013.

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Patents

[20] Ramjugernath D., Williams-Wynn M., Čárský M., Heyberger A., Gruber V.: Recovery of Yttrium and Europium Compounds. *Pat. No. ZA 2013/02663*. Applied: 13.04.15.

[21] Petričkovič R., Uchytil P., Řezníčková J., Setničková K., Storch J.: Způsob separace plynu ze směsi plynů. (Czech) bude. Pat. No. PV 2012-725. Applied: 12.10.25.

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PHD STUDENTS
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Fields of research

- Thermophysical properties of pure ionic liquids and their liquid phase behavior in mixtures with molecular solvents
- Experimental determination of vapor–liquid equilibria in mixtures containing components of low and high molecular mass
- Data processing with activity coefficient models and equations of state
- Prediction of phase behavior using models based on group contribution methods
- 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
- Molecular simulations of ionic 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

Applied research

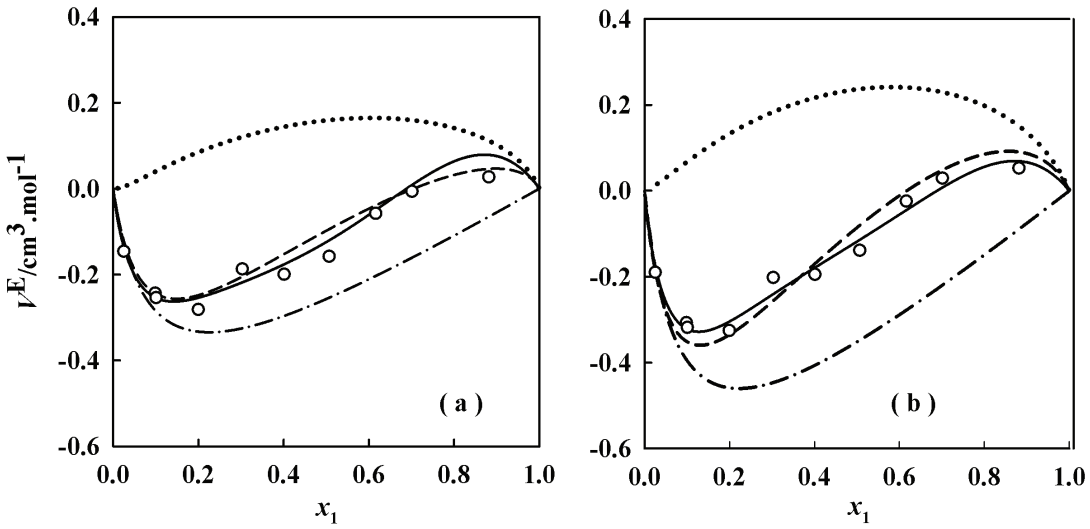
- Technology for the preparation of molecularly imprinted polymeric materials – Project: *Novel technology of molecularly imprinted polymeric materials preparation*, MoSES Republic of Croatia (2007–2014)

Research projects

Excess molar volumes and excess molar enthalpies in binary systems N-alkyl-triethyl-ammonium bis{(trifluoromethyl)sulfonyl}imide + methanol [1]

(M. Bendová, bendova@icpf.cas.cz; joint project with QUILL Belfast, UK and Laboratory of Thermophysics, Department of Applied Physics, Universidade de Vigo, supported by ICPF)

A study on the influence of the alkyl chain length in N-alkyl-triethylammonium bis{(trifluoromethyl)sulfonyl}imide ionic liquids, $[N_{R,222}][Tf_2N]$ (R = 6,8 or 12), on the excess molar enthalpy at 303.15 K and excess molar volume within the temperature interval (283.15–338.15 K) of ionic liquid + methanol mixtures was performed. Small excess molar volumes with highly asymmetric curves (i.e. S-shape) as a function of mole fraction composition were obtained, with negative values showing in the methanol-rich regions. The excess molar volumes increase with the increase of the alkyl-chain length of the ammonium cation of the ionic liquid and decrease with temperature. The excess enthalpies of selected binary mixtures are positive over the whole composition range and increase slightly with the length of the alkyl side-chain of the cation on the ionic liquid. Both excess properties were subsequently correlated using a Redlich–Kister-type equation, as well as by using the ERAS model. From this semipredictive model the studied excess quantities could be obtained from its chemical and physical contribution. Finally, the COSMOThermX software has been used to evaluate its prediction capability on the excess enthalpy for investigated mixtures at 303.15 K and 0.1 MPa. From this work, it appears that COSMOThermX method predicts this property with good accuracy of approx. 10%, providing at the same time the correct order of magnitude of the partial molar excess enthalpies at infinite dilution for the studied ILs $\overline{H}_1^{E,\infty}$, and methanol, $\overline{H}_2^{E,\infty}$.



Excess molar volume in system $[N_{6,222}][Tf_2N]$ (1) + methanol (2) at T = 298.15 K (a) and T = 328.15 K (b). (○) experimental data; full line – Redlich-Kister expansion; dash line – ERAS prediction; dotted line – ERAS chemical contribution; dash-dotted line – ERAS physical contribution

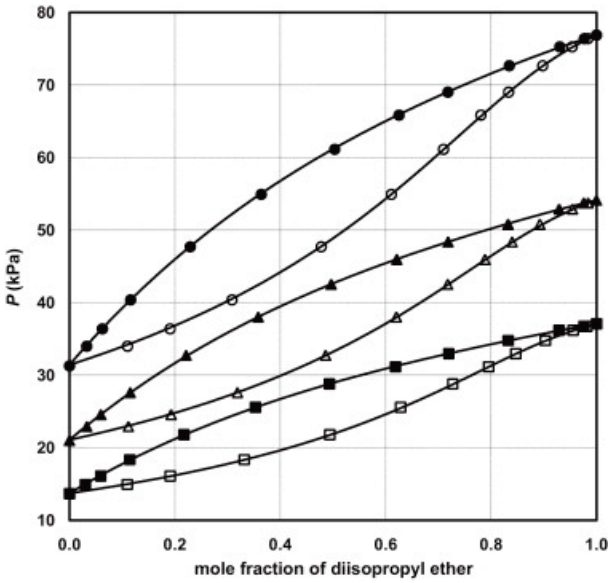
[1] Machanová, K.; Troncoso, J.; Jacquemin, J.; Bendová, M. *Fluid Phase Equilibria*, paper in press as of December 2013

Vapour − liquid equilibrium – measurement and data processing

(I. Wichterle, wichterle@icpf.cas.cz supported by ICPF)

a) Systems containing low molecular mass components

Isothermal vapour−liquid equilibrium data were measured in there binary and one ternary systems containing alcohol, ether and ketone. [Ref. 16]

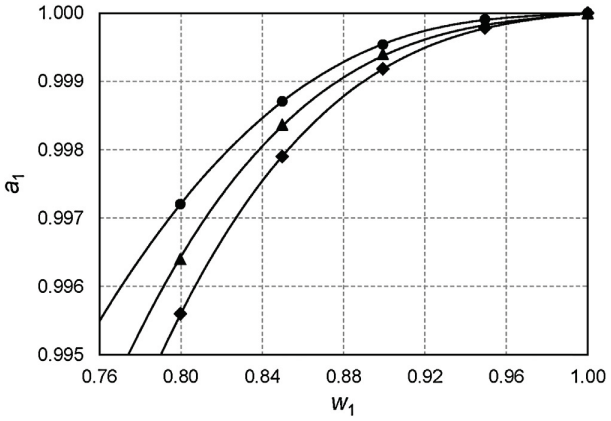


Isothermal vapour – liquid equilibrium in the diisopropyl ether + 3-methyl-2-butanone system (*x*–*y*–*P* plot). Experimental data: 313.15 K (■, □), 323.15 K (▲, △), 333.15 K (●, ○); (solid points) liquid phase; (open points) vapour phase; (—) NRTL correlation

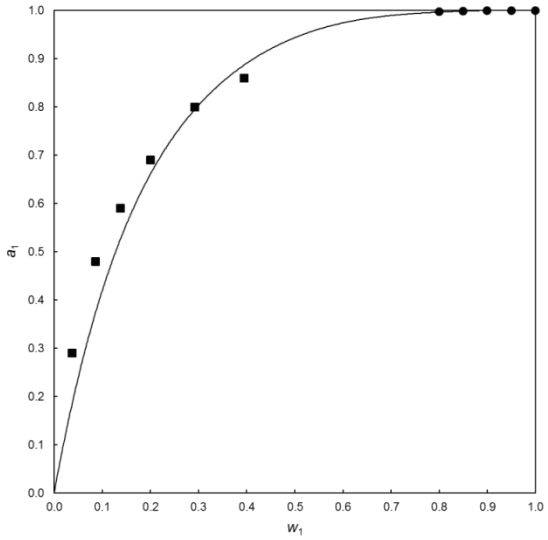
b) Systems containing polymers

Vapour–liquid equilibria have been determined in systems composed of poly(acrylic acid) with water, and poly(methyl methacrylate) with acetone by ebulliometric (total pressure measurement) method. Ebulliometer has been redesigned and experimental procedure has been upgraded. Experiments have been carried out isothermally, the measured data were correlated by the UNIQUAC equation, 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 ICPF. Results were published in journal [17] and presented at 13th International Conference on Properties and Phase Equilibria for Products and Process Design, Iguazu Falls, Argentina.

Microebulliometer – new design



Activity a_1 of water in PAA as a function of water mass fraction w_1.
Experimental data at (●) 353.15 K;
(▲) 363.15 K and (◆) 373.15 K.
Solid lines represents correlated activities using the UNIQUAC model at 353.15, 363.15 and 373.15 K



Activity a_1 of water in PAA as a function of water mass fraction w_1.
Experimental data at (●) 353.15 K [ref. 17], (—) correlated activities using the UNIQUAC model at 353.15 K; experimental data at (■) 303.15 K [Arce A., Fornasiero F., Rodrigues O., Radke C.R., Prausnitz J.M., Phys. Chem. Chem. Phys. 6, 103-108 (2004)].

c) Prediction of properties of petroleum fluids

A simplified method for characterizing petroleum fluids (crude oil and gas condensate) and for predicting phase equilibria developed earlier was presented as invited lecture at World Congress on Petrochemistry and Chemical Engineering, San Antonio, USA and at 38th Croatian Invention Exhibition with International Participation, INOVA 2013, Zagreb, Croatia.

Molecular-level simulations aqueous electrolytes

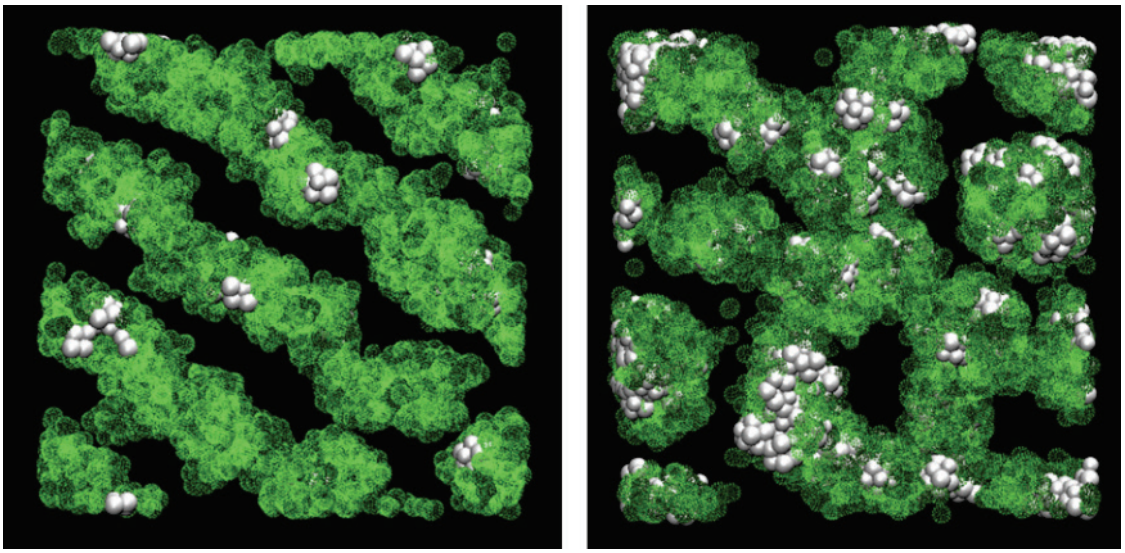
(I. Nezbeda, ivonez@icpf.cas.cz, joint project with the University of Ontario, Institute of Technology, Oshawa, ON, Canada and UJEP; supported by UJEP)

This series of papers deals with common non-polarizable models of electrolytes with the goals to (i) assess their appropriateness, (ii) find ranges of their applicability, and (iii) examine the possibility of their improvement by a reparametrization. Consistency tests of available literature data for the chemical potential were also performed. All simulations used the recently developed MPM-MC method demonstrating thereby its efficiency. [Refs. 10-13]

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. [Ref. 18]



Effect of nanofiller loading in a PS_2PVP_{18} (f = 0.1). *PS* domain is represented as dotted green spheres and *NPs* as white spheres. *PVP* domain is omitted for clarity

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. 5-7, 15]

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. 3, 4]

International co-operations

Imperial College London, London, UK: Confined fluids

INA, Research and Development, Zagreb, Croatia: Novel technology of molecularly imprinted polymeric materials preparation

Penn State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behavior of model proteins on surface

Queen's University Ionic Liquids Laboratory (QUILL), Belfast, UK: Liquid–liquid phase equilibria in systems of ionic liquids
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
Wrocław University of Technology, Department of Chemical Engineering, Poland: Solubility behavior of chiral ionic liquids in water and 1-octanol, and their tendency to bioaccumulation
Laboratoire TIM, Institut de chimie de Clermont-Ferrand, CNRS UMR 6296 / Université Blaise Pascal, France: How the presence of a molecular component will affect the structure, interactions and ionicity of an ionic liquid?
Laboratory of Thermophysics, Department of Applied Physics, Universidade de Vigo, Spain: Excess molar properties in systems of ionic liquids with methanol

Visits abroad

M. Lísal: Pennsylvania State University, State College, PA, USA (1 month)
A. Malijevský: Imperial College London, London, UK (3 months)
A. Malijevský: University of Loughborough, Loughborough, UK (2 weeks)

Visitors

A. Archer, University of Loughborough, Loughborough, UK
C. Hardacre, Queen's University Ionic Liquids Laboratory (QUILL), Belfast
J. Jacquemin, Queen's University Ionic Liquids Laboratory (QUILL), Belfast
J. Troncoso, Laboratory of Thermophysics, Department of Applied Physics, Universidade de Vigo
B. Rathke, Faculty of Engineering, Bremen University
J. Feder-Kubis, Department of Chemical Engineering, Faculty of Chemistry, Wrocław University of Technology

Teaching

M. Bendová: ICT, Faculty of Chemical Engineering, postgraduate course "Physical Chemistry for Technological Practice"
J. Jirsák: UJEP, Faculty of Science, courses "Introduction to Chemistry", "Physical Chemistry", "Physical Chemistry Seminar" and "Free Software in Natural Sciences"
M. Kotrla, M. Předota: CU, course “Advanced Computer Simulations in many Particle Systems”
M. Lísal: UJEP, Faculty of Science, courses “Parallel Programming”, “Numerical Mathematics”, “Molecular Simulations” and “Mesoscale Simulations”
A. Malijevský: ICT, Faculty of Chemical Engineering, courses “Physical Chemistry I”, “Physical Chemistry of the Micro-World", "Introduction to a Modern Theory of Phase Transitions", "Mathematics for Physical Chemistry" and "Statistical Thermodynamics"
M. Předota: University of South Bohemia, České Budějovice, courses “Lectures from Physics Oriented to Particle and Nuclear Physics” and “Selected Lectures from Physics”

Publications

Original papers

[1] Houšková H., Morávková L., Sedláková Z., Boublík T., Kolská Z.: Volumetric Behavior of the Ternary System Benzene – 2-Methoxy-2-Methylbutane – 2,2,4-Trimethylpentane and All Binary Sub-Systems at Temperature Range (298.15 – 318.15) K. *Fluid Phase Equil.* 337, 156-164 (2013).

[2] Kárászová M., Šimčík M., Friess K., Randová A., Jansen J.C., Růžička M., Sedláková Z., Izák P.: Comparison of Theoretical and Experimental Mass Transfer Coefficients of Gases in Supported Ionic Liquid Membranes. *Sep. Purif. Technol.* 118, 255–263 (2013).

[3] Lísal M.: The Liquid Surface of Chiral Ionic Liquids as Seen from Molecular Dynamics Simulations Combined with Intrinsic Analysis. *J. Chem. Phys.* 139(21), 214701-15 (2013).

[4] Lísal M., Izák P.: Molecular Dynamics Simulations of n-Hexane at 1-Butyl-3-Methylimidazolium bis(trifluoromethylsulfonyl) Imide Interface. *J. Chem. Phys.* 139(1), 014704 (2013).

[5] Lísal M., Předota M., Brennan J.K.: Molecular-Level Simulations of Chemical Reaction Equilibrium and Diffusion in Slit and Cylindrical Nanopores: Model Dimerization Reactions. *Mol. Simul.* 39(13), 1103-1120 (2013).

[6] Malijevský A., Parry A.O.: Density Functional Study of Complete, First-Order and Critical Wedge Filling Transitions. *J. Physics-Condensed Matt.* 25(30), 305005 (2013).

[7] Malijevský A., Parry A.O.: Critical Point Wedge Filling. *Phys. Rev. Lett.* 110(16), 166101 (2013).

[8] Morávková L., Troncoso J., Machanová K., Sedláková Z.: Volumetric Behaviour of the (2,2,4-Trimethyl-pentane + Methylbenzene + Butan-1-ol) Ternary System and Its Binary Sub-Systems within the Temperature Range (298.15–328.15) K. *J. Chem. Thermodyn.* 64, 137–150 (2013).

[9] Moučka F., Nezbeda I.: Gibbs Ensemble Simulation on Polarizable Models: Vapor-liquid Equilibrium in Baranyai-Kiss Models of Water. *Fluid Phase Equilib.* 360, 472-476 (2013).

[10] Moučka F., Nezbeda I., Smith W.R.: Computationally Efficient Monte Carlo Simulations for Polarizable Models: Multi-Particle Move Method for Water and Aqueous Electrolytes. *Mol. Simul.* 39(14-15), 1125-1134 (2013).

[11] Moučka F., Nezbeda I., Smith W.R.: Molecular Force Field Development for Aqueous Electrolytes: 1. Incorporating Appropriate Experimental Data and the Inadequacy of Simple Electrolyte Force Fields Based on Lennard-Jones and Point Charge Interactions with Lorentz-Berthelot Rules. *J. Chem. Theory Comput.* 9(11), 5076-5085 (2013).

[12] Moučka F., Nezbeda I., Smith W.R.: Molecular Simulation of Aqueous Electrolytes: Water Chemical Potential Results and Gibbs-Duhem Equation Consistency Tests. *J. Chem. Phys.* 139(12), 124505-7 (2013).

[13] Moučka F., Nezbeda I., Smith W.R.: Molecular Force Fields for Aqueous Electrolytes: SPC/E-Compatible Charged LJ Sphere Models and Their Limitations. *J. Chem. Phys.* 138(15), 154102-9 (2013).

[14] Nezbeda I., Rouha M.: Extended Excluded Volume: Its Origin and Consequences. *Pure. Appl. Chem.* 85(1), 201-210 (2013).

[15] Pařez S., Guevara-Carrion G., Hasse H., Vrabec J.: Mutual Diffusion in the Ternary Mixture of Water Plus Methanol Plus Ethanol and Its Binary Subsystems. *Phys. Chem. Chem. Phys.* 15(11), 3985-4001 (2013).

[16] Pavlíček J., Andresová A., Bogdanić G., Wichterle I.: Vapour–Liquid Equilibria in the Binary and Ternary Systems Composed of 2,3-Dimethylbutane, Diisopropyl Ether, and 3-Methyl-2-Butanone at 313.15, 323.15 and 313.15 K. *Fluid Phase Equilib.* 344, 59-64 (2013).

[17] Pavlíček J., Bogdanić G., Wichterle I.: Vapour–Liquid Equilibria in the Polymer + Solvent System Containing Lower Concentrations of Solute at Normal or Reduced Pressures. *Fluid Phase Equilib.* 358, 301-303 (2013).

[18] Posel Z., Posocco P., Fermeglia M., Lísal M., Pricl S.: Modeling Hierarchically Structured Nanoparticle/Diblock Copolymer Systems. *Soft Matter* 9(10), 2936-2946 (2013).

Review papers

[19] Morávková L., Sedláková Z.: Excess Molar Volume of Binary Systems Containing Mesitylene. *Kemija u industriji* 62(5-6), 159-170 (2013).

[20] Wichterle I.: Editorial. *Kemija u industriji* 62(5-6), 2 (2013).

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Fields of research

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

Applied research

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

Research projects

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

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

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

During the UCG process as well as a long time after the process termination a great number of hazardous environmental contaminants (both inorganic and organic species) can be released into the groundwater environment. Within this project, the solute transport processes in groundwater were modeled using the saturated zone model of groundwater flow including phenomena that incorporates advection, both mechanical and hydrodynamic dispersion, solute diffusion as well as adsorption of solutes on the rock inner surfaces. Used model was formulated under consideration of the rock saturation with water. Water fills completely all volume of voids in porous rocks and creates a saturation zone. From a mathematical point of view, the model description takes into consideration Darcy's law, Fick's law of diffusion and equation of adsorption isotherms.

Fly ash from coal combustion have been chosen as potentially best fill material for filling of UCG voids and control of release and migration of contaminants due their widely known ability to isolate contaminants, between other in landfilling, beneficial physical properties and availability. From the point of the view of isolation of contaminants a very important factor is the filtration coefficient of solidified (stabilized) fly ash – water mixtures, what become subject of laboratory measurements. [Ref. 26]

Pilot reactor with reactive barrier made by active carbon after 5 days processing

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.

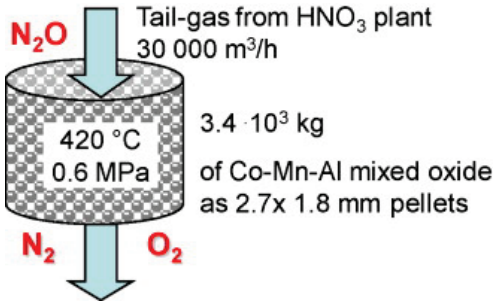
Therefore, the main objective of the project is to develop a family of advanced nano- and ultrafiltration ceramic composite membranes containing functionalized mesoporous silica layers which will be capable of selective binding of heavy metals (Hg, Cd, Cr) and uranium from surface and waste waters and thus preventing or minimizing the environmental exposure to hazardous substances. [Ref. 24]

Abatement of N_2O emissions in off-gas from nitric acid technology

(K. Jirátová, jiratova@icpf.cas.cz; joint project with TU of Ostrava, and ICT; supported by TACR, project No. TA01020336)

Alkali promoted Co_4MnAlO_x mixed oxide (molar ratio of alkali metal/Co = 0.037) were prepared by impregnation of calcined Co-Mn-Al hydrotalcite (molar ratio Co : Mn : Al = 4:1:1) with an aqueous solution of Li, Na, K, Rb or Cs nitrate. N_2O conversion over alkali promoted Co_4MnAlO_x mixed oxide decreased in order Cs > Rb > K > Na = Co_4MnAlO_x > Li in inert gas and was shifted to the lower values in the presence of typical components (NO_x, O_2 and H_2O) of flue gas. The addition of alkali promoters to the Co_4MnAlO_x mixed oxide resulted in a modification of both electronic properties of active metals and acid-base function of the catalyst surface. The promotional effect of alkali metals is connected with their ionization potential, the charge transfer to the catalyst and a decrease in binding energies of all catalyst components (Co, Mn, Al and O). Pilot plant verification of N_2O decomposition over K-promoted Co_4MnAlO_x is shown.

A catalyst for N_2O removal from effluents of nitric acid plants was patented. The catalyst consists of calcined beta-cobalt hydroxide and Cs. The catalyst is prepared by action of NaOH on cobalt nitrates solution in molar NaOH / $Co(NO_3)_2$ = 0.5 to 2.0 at 20 to 25 °C under mixing for 5-10 min, then is dried, formed into pellets, calcined and impregnated with water solution of Cs compounds to meet molar ratio Cs to Co_3O_4 in the range from 0.003 to 0.060 and again is calcined. Concentration of N_2O in the treated gas is lower than 150 ppm, when initial concentration of N_2O is 1000 ppm and GHSV 0.001 g min ml^{-1}. [Refs.19, 31]

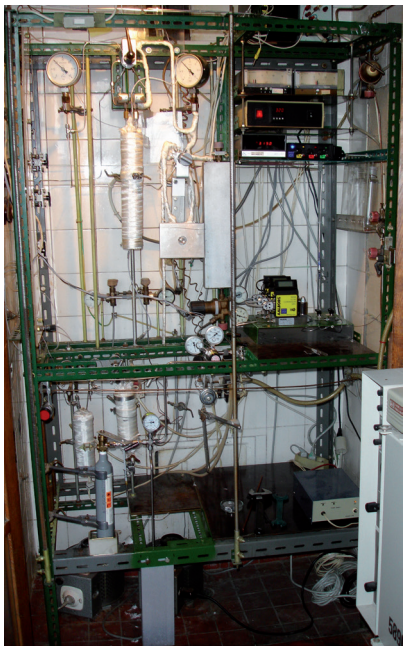


Scheme of the reactor arrangement for N_2O decomposition

Study of hydrodesulfurization and its inhibition by hydrogenation (denitrogenation) over catalysts containing small amounts of noble metals

(Z. Vít, vit@icpf.cas.cz; joint project with Department of Chemistry, Physics and Environment, University of Udine, Italy; supported by GACR, project No. 104/09/0751)

Acidic supports and active phases containing noble metals were studied for hydrodesulfurization (HDS) of model compounds such as thiophene and benzothiophene. Silica-alumina's modified by post-synthesis acid extraction were studied as possible supports of bimetallic Pd-Pt catalysts. The extraction of support increased the surface areas and exposed more Brønsted acidic sites which improved the HDS activity of catalysts. HDS activity was greatly affected by metal precursor and the way of catalyst pretreatment. It was shown that a fraction of active phase, enriched by Pd, accumulated hydrogen in the form of β-Pd hydride phase. Amounts of hydrogen held by hydride phase correlated with thiophene HDS activities showing that activated hydrogen participated in HDS. The inhibition effects of pyridine and quinoline on HDS of thiophene and benzothiophene were studied on Mo and Pd-Mo/alumina catalysts. Noble metal containing catalysts were generally less sensitive to nitrogen bases than conventional CoMo catalysts. Activities and nitrogen tolerance were in relation to C-N bond breaking activity of nitrogen inhibitor.



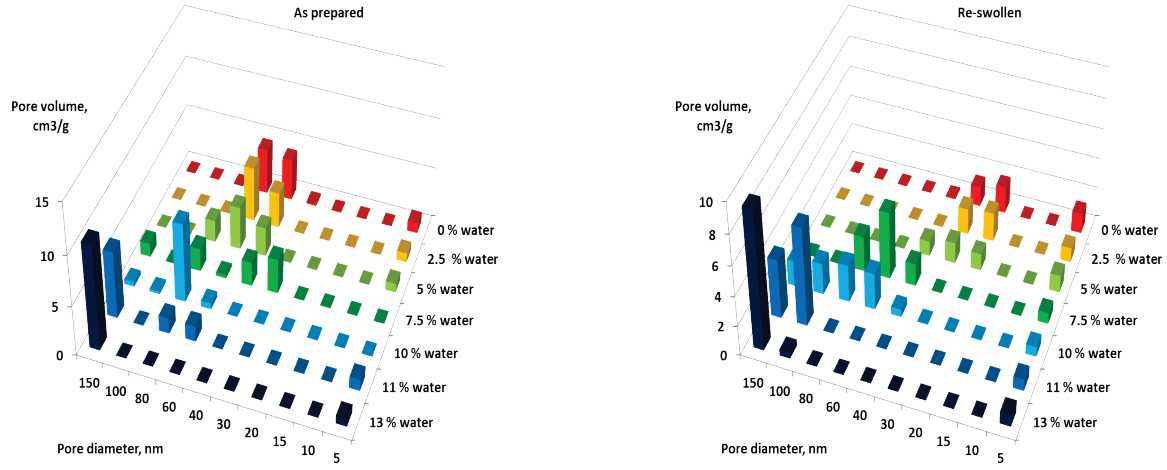
Pressure flow microreactor with fixed bed of catalyst for hydrodesulfurization

Morphology and application properties of mesoporous poly(divinylbenzenes)

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

Chinese colleagues discovered a novel polymerization method producing porous polymers with very high surface area and unique mesoporous morphology, completely different from conventionally prepared materials of similar chemical nature. In their preparation is used exceptionally high dilution of monomers with porogenic solvents. With help of inverse steric exclusion chromatography method developed in Prague providing information on the polymer morphology in its native, swollen state undeformed are investigated relations between preparation conditions of mesoporous functional polymers and their morphology and applications for which the exceptional properties of the mesoporous functional polymers could be advantageous. It was found that the pore volume in the polymer examined just after preparation corresponded to the volume of the porogen used. Resulting high porosity exceeding 90 % can be explained only on the basis of pore formation through

microsyneresis rather than the macrosyneresis mechanism that is common in the synthesis of conventional porous polymer materials. Drying of the polymers of course induces extensive collapse of the porous structure. Water, as additive to the porogenic solvent, influences ability of the polymer morphology to re-swell to its original state.

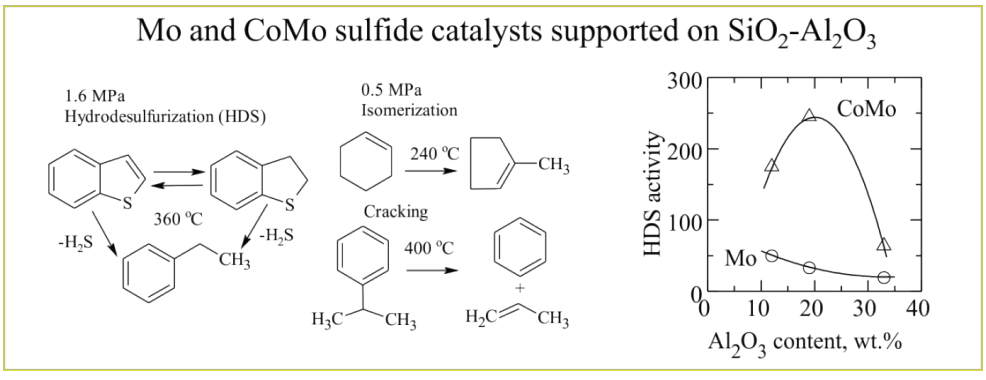


Influence of addition of water to porogenic solvent on the swollen-state morphology of mesoporous poly(divinylbenzenes

Unconventional composition and preparation of sulfide hydrotreating catalysts

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

Catalysts with various MoO_3 and Al_2O_3 contents were prepared by a reaction of acidic SiO_2-Al_2O_3 supports with aqueous slurry of MoO_3. The saturated adsorption amount of MoO_3 corresponded with the amount of Al_2O_3 in the supports. The deposited and sulfided Mo species were accessible for promotion of the activity and selectivity in benzothiophene hydrodesulfurization reaction by Co. The acidity of the SiO_2-Al_2O_3 supports modified by dealumination by leaching with nitric acid in terms of cyclohexene isomerization and cumene cracking were preserved after deposition of the CoMo sulfide phase. Furthermore, a new method based on impregnation of unconventional supports (i.e. activated carbon and ZrO_2) by the nitrilotriacetic acid (NTA) assisted spreading of molybdenum trioxide with cobalt carbonate, or ammonium heptamolybdate with cobalt carbonate was investigated. The NTA systematically increased the promotion effect of Co in the sulfided catalysts in comparison to samples prepared without NTA from ammonium heptamolybdate and cobalt nitrate. The promotion effect of Co was expressed as ratio of activity of CoMo catalyst and its Mo counterpart and NTA increased it by the factor 1.13-1.58 for the studied supports. [Refs. 8, 9]



Model hydrotreaning reactions for unconventional catalysts

Microalgaes as a promising sources 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 ASCR, Mydlářka a.s., Rabbit CZ a.s., Rabbit Chotýšany a.s., CU, ICPF, ICT 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 biotechnologically produced eustigmatofit microalgaes with the high content of PUFA, have been applied. New types of mixotrophic bioreactors were designed to obtain the optimal content PUFA in biomass. Products will be used as the feeding additives for poultry.

The newly designed biophotoreactor

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)

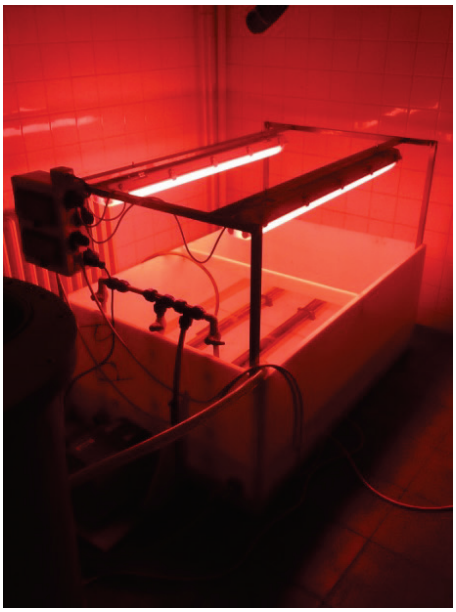
Fulfilling of increasingly stringent environmental restrictions imposed on transportation drives the research on alternative energy resources such as hydrogen and fuel cells. Preparation of carbon black supported 60 wt. % Pt was studied as a conventional catalyst for membrane electrode assembly. Platinum was deposited on the supports XC72R, XC72 (Vulcan, Cabot Corp.), and ENSACO 290G, 350G (Timcal Graphite & Carbon Ltd.) and a research grade PT-P (Timcal Graphite & Carbon Ltd.): (i) from true solutions of H_2PtCl_6, $Pt(C_5H_7O_2)_2$, $Pt(NH_3)_4(NO_3)_2$, or $Pt(NH_3)_2(NO_2)_2$, and (ii) from fine dispersions of $Pt(C_5H_7O_2)_2$, PtO_2, $Pt(NH_3)_4(OH)_2$. Atomic adsorption spectroscopy and scanning electron microscopy were used for elemental analysis and determination of Pt content. N_2 adsorption-desorption measurements revealed highly developed mesoporous system with maximum on the pore-size distribution curve at pore-size radius 7 nm for Pt-P, which was quite unique among the studied supports. Deposited Pt species were dried, calcined or reduced and were subjected to temperature programmed reduction (TPR). After degassing at increased tempera-

ture, the Pt dispersion was determined by hydrogen chemisorption at - 60 °C. TPR revealed that PtO_2, H_2PtCl_6, $Pt(C_5H_7O_2)_2$, $Pt(NH_3)_4(NO_3)_2$, and $Pt(NH_3)_2(NO_2)_2$ deposited on carbon blacks and dried in rotary vacuum evaporator at 95 °C were reduced to metallic Pt at 0, 70, 120, 140, 150 °C, respectively. Specific interaction of the Pt precursor with support surface was considered necessary for formation of the desired 4-6 nm Pt particles from H_2PtCl_6 or $Pt(NH_3)_2(NO_2)_2$. The deposition of colloidal form of PtO_2 or $Pt(C_5H_7O_2)_2$ seemed to be particularly promising because it represented relatively clean and gentle method of Pt deposition. This was manifested by the sharp reduction peaks but the tailored high Pt dispersion was not reached.

Reactive chemical barriers for decontamination of heavily polluted waters

(P. Klusoň, kluson@icpf.cas.cz; joint project with Dekonta a.s.; supported by MIT, project No. FR-TI1/065)

The project was focusing on the final studies of the special oxidations of contaminants in industrially polluted waters. Special attention was paid to aniline and nitrobenzene waters, to waters with dissolved chlorinated compounds and to inorganic contamination with certain specific ions. The used methods were the photocatalytic oxidations with phthalocyanines, name with Zn phthalocyanine, and with UVC and hydrogen peroxide. Among other techniques electrocoagulation was also tested to reduce both the organic as well as the inorganic pollutants. The project thus deals in a complex manner with the problem of industrial pollution of various types and origins. The Recheba concept represents a kind of passive approach, however, assisted with highly advanced processes for effective water decontamination. The systems had been still tested on a laboratory scale, however, much more attention was now paid to the large scale operations. [Ref. 30]



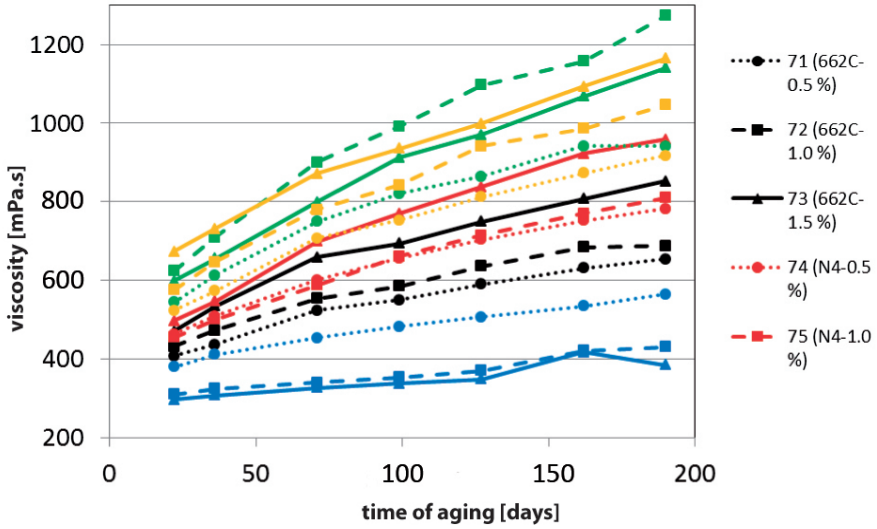
Detail of the phthalocyanine decontamination unit

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

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

This project deals with utilization of special types of ionic liquids based on tetra-alkylammonium 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.



Viscosity change (at T = 23°C) in time of alkyde resin with various ionic liquids at three concentrations (additives do not change the Newtonian character of resin)

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

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

Aim of the project, shortly named *Color Clocks,* focuses on the applied research & development and testing of the advanced thin film elements for direct evaluation of the time variable by means of preciously calibrated color change. These elements represent a highly specific form for time measurement under highly specific conditions and for very specific practical purposes. These structures are supposed to be used as tools for simple visual and intuitive evaluation of the time variable under very different circumstances. It is a kind of standard memory element collecting a certain type of data, which are then assessed in the cumulative form as the absorbed light dose of characteristic energy, or characteristic energetic region. The light sensitive films are based on uniformly organized nanoparticles that exhibit an adjustable photocatalytic activity toward the decomposition of selected organic structures deposited onto their surfaces. The decolorization process is then carefully calibrated for many different types of probe organic molecules. There are many possible practical applications of these materials, among others dermatology, conservation and storage of historical monuments and artefacts, should be mentioned.

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

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

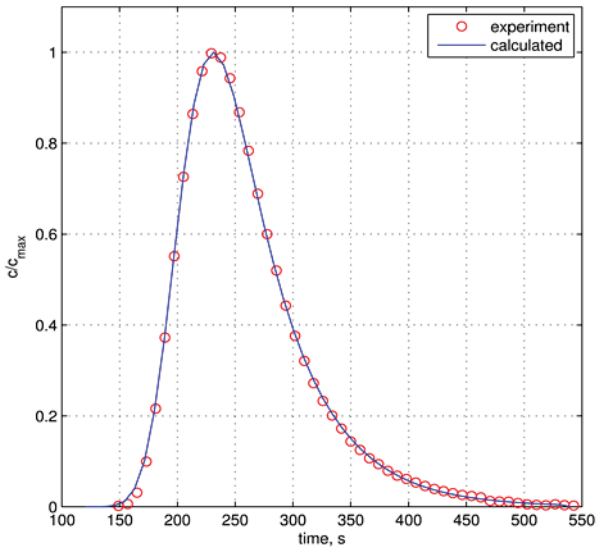
Searching after the functional relationship between diffusion of fluid in disordered solids (e.g. porous solids) and their microstructure is an active field of research in membrane scien-

ce, catalysis, biophysics, civil engineering and other branches of research and development. During several past decades the pulsed field gradient (PFG) NMR technique has proved to be a powerful tool for measuring of self-diffusion in such systems. The focus of the project is on transport investigation of liquid species contained in porous materials (non-consolidated and consolidated) with monodisperse and bidisperse porous structure with excursions to adjacent supercritical regions. A rational system of transport-related structure characteristics to predict transport behavior of liquids and supercritical fluids will be searched by combined application of PFG NMR, image analysis of porous materials and molecular simulation of self-diffusion in selected two-phase systems.

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

The effective diffusion coefficients for two polystyrene samples with different relative molecular weights (1000 and 100,000) in cyclohexane on hydroxyapatite were evaluated Comparison of the chromatographic response signals for polystyrene tracers with different molecular weights is depicted in Fig. Furthermore, Fig. illustrates a very good fit between experimental data (circle marks) and the calculated chromatographic response signals (solid lines) based on the optimized model parameters.

It was found that the binary effective diffusion coefficients revealed much lower values in comparison with the binary bulk ones due to the strong influence of hindered diffusion in hydroxyapatite pore network. [Refs. 25, 29].



Response curve for polystyrene (M_w = 100,000) in cyclohexane on hydroxyapatite. Experimental (°), calculated (—)

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

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

Endocrine disruptors represent the group of chemical substances disrupting the hormonal indication of vertebrates and thereby they could encroach on the organism function. To the group of endocrine disruptors belong surfactants, softeners, fungicides, insecticides and some kinds of medications and hormonal contraception. They are commonly presented not only in

the waste water but also in the natural water. Endocrine disruptors are persistent to degradation by common chemicals as well as biological and photolytic processes. The necessity of finding the alternative solutions leads to development and use of the new technologies. Photo-catalysis using semiconductor particles have found increasing interest to solve the endocrine disruptors remove problems.

This study is focused on verification of the specially designed photoactive materials and their modified versions suitable for photo-processes carried out upon illumination in the UV-light. Ethynylestradiol, nonylphenol and bisphenol A were chosen as typical compounds belong to the endocrine disruptor group. In this work the water decontamination with various concentrations of endocrine disruptors in the two types of reactors; batch and plug flow arrangement on the titania thin layers were studied. Moreover, the application of the specially designed pilot plan photoreactor has been studied. [Ref. 16]

Pilot plant photo-reactor

Ionic liquids as additives for special pigments

(O. Šolcová, solcova@icpf.cas.cz; joint project with Synthesia, Techem; supported by MIT, project No. FR-TI4/189)

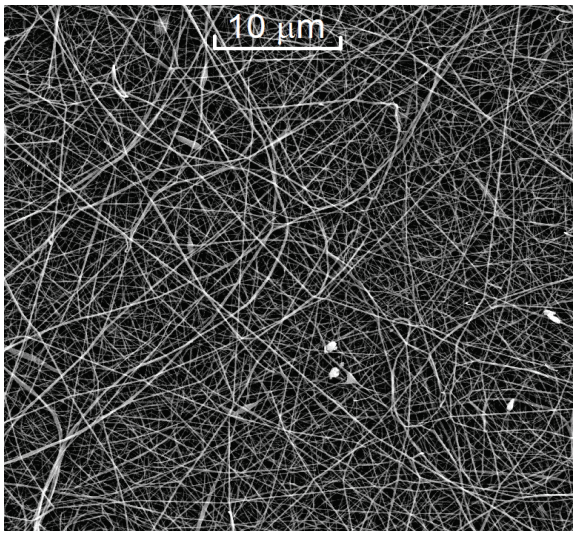
Ionic liquids are composed of large ions with a low degree of the overall molecular symmetry. Very high coloumbic interactions are behind their impressive electrical and mechanical stabilities, thermal and pressure resistivity, and extremely low tension of vapors. Low flammability, very good electrical conductivity, high thermal capacity and unusual phase behavior might be added to the previous list of exceptional properties. No doubts these features qualify them for a broad band applications ranging from “green solvents” due to their negligible volatility, over templates for synthesis of nanoparticles (some of them tend to form organized ionic clusters), liquid electrolytes in solar cells and fuel cells, to liquid adhesives, special lubricants, chromatography mobile phases, incombustion additives, etc.

One of the most prominent applications is their use as special additives for pigments and dye compositions. If the side-chains are too short, they do not disturb the ionic network significantly and, also, they do not possess enough conformational freedom to adopt a low energy configuration. However, increasing the chain-length the role of its spatial arrangement becomes much more important. In this respect this project pays special attention to the utilization of quartenary ammonium ionic liquids, namely n-alkyl-triethylammonium bis(trifluoromethane sulfonyl) imides ($N_{R222}Tf_2N$, R = 6, 7, 8, 10, 12, 14) with a variable length of an alkyl chain are specially promising.

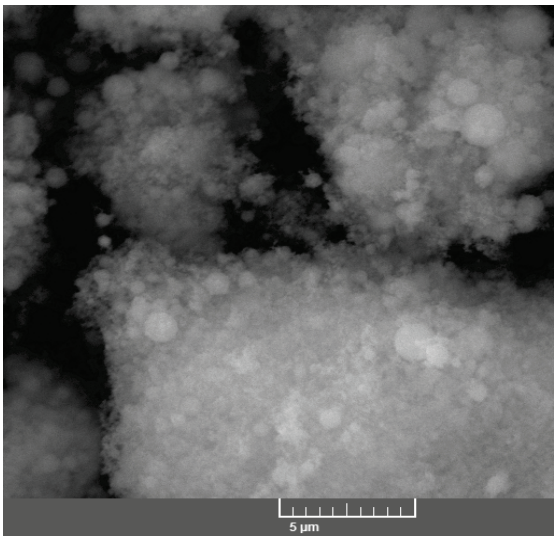
Transport characteristics of novel biocompatible materials

(K. Soukup, soukup@icpf.cas.cz; supported by GACR, project No. P106/11/P459)

The aim of the project was focused on comprehensive characterization of the microstructure properties of the novel biocompatible porous solids included both electrospun polymeric membranes and bone-like hydroxyapatites. In order to prepare materials having the targeted effects for the required applications (both in medical and chemical), the knowledge of the transport characteristics typical of its pore network is of the prime importance. Four experimental setups were utilized for the transport characteristics determination: Graham's diffusion cell, Wicke-Kallenbach cell, and permeation cell were used for the gas transport measurements and inverse liquid chromatography technique for diffusion measurements in liquids. Special attention was paid to the detailed statistical analysis of the optimized transport parameters and effective binary diffusion coefficients. The statistical reliability of the calculated transport parameters was assessed by means of their confidence regions (from diffusion measurements) and confidence intervals (from permeation measurements) computed at a significance level of 5%. It was found that the confidence of the optimized transport parameter ψ (from diffusion) and $\langle r \rangle \psi$ (from permeation) reflecting the influence of the molecular and Knudsen mass transport mechanism, respectively, was much higher than transport parameters $\langle r \rangle \psi$ (from diffusion) and $\langle r^2 \rangle \psi$ (from permeation). It was additionally found that tracer solute with the larger molecular weight shows shorter retention time compared to tracer solute with the lower molecular weight. The observed difference in retention times corresponds to expectation that the short-chain solute will penetrate deeper to the pore system of biocompatible nanopowders and will be more retained in comparison with the long-chain solute. [Refs. 25, 26, 29]



Micrograph of nanofibrous chitosan



Micrograph of bone-like hydroxyapatite

New heterogeneous catalysts for environmental protection

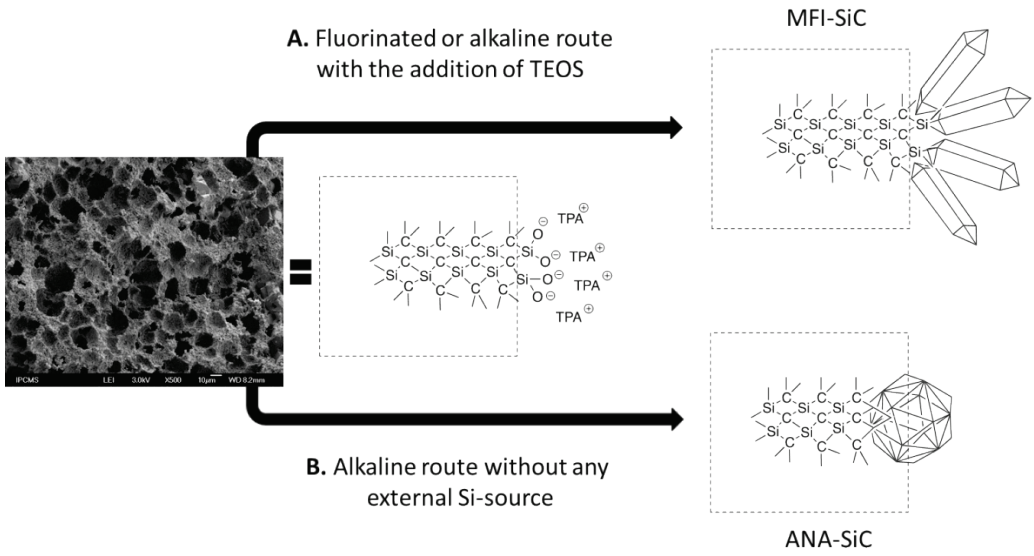
(L. Kaluža, kaluza@icpf.cas.cz; joint bilateral co-operation with Institute of Catalysis, BAS, Sofia, Bulgaria; supported by ASCR)

High surface area TiO_2 nanotubes (Ti-NT) synthesized by alkali hydrothermal method were used as a support for NiW hydrodesulphurization catalyst. Nickel salt of 12-tungstophosphoric acid ($Ni_{3/2}PW_{12}O_{40}$) was applied as oxide precursor of the active components. A polytungstate phase evidenced by Raman spectroscopy was observed indicating the destruction of the initial heteropolyanion. The catalytic experiments revealed two times higher thiophene conversion on NiW catalyst supported on Ti-NT than those of catalysts supported on alumina and titania. Increased HDS activity of the NiW catalyst supported on Ti-NT could be related to a higher amount of W oxysulfide entities interacting with Ni sulfide particles as consequence of the electronic effects of the Ti-NT observed with XPS analysis. [Ref. 20]

Novel materials with hierarchical pore structure: preparation and evaluation of the transport characteristics

(K. Soukup, soukup@icpf.cas.cz; joint bilateral project with University of Strasbourg;
supported by MEYS, project No. 7AMB12FR029)

In the present bilateral project, we would like to propose strategies towards the design of structured catalytic beds made of hierarchical zeolites with improved hydrodynamics (compared to extrudates or conventional pellets), combining both the advantages of zeolitic catalysts and of a tailored porosity (triple level of porosity: micro-, meso- together with an appropriate macroporosity). Several syntheses have been performed to allow the growth of zeolite crystals on α-silicon carbide supports (α-SiC). Silicon-carbide foams exhibit a duplex macroporous structure. Framework type MFI and ANA of zeolites have been successfully coated to this relatively inert supporting material. While the synthesis of MFI/SiC required the presence of an additional Si-containing source, in contrast, ANA/SiC composites have been unexpectedly obtained through the self-recrystallization of the silicon contained in the α-SiC substrate. The different composite materials were thoroughly characterized by SEM, comprehensive textural and gas transport measurements and XRD. The coating rates as well as the coverage by ANA zeolite crystals on SiC surface were determined by both SEM observations and nitrogen physisorption measurements.

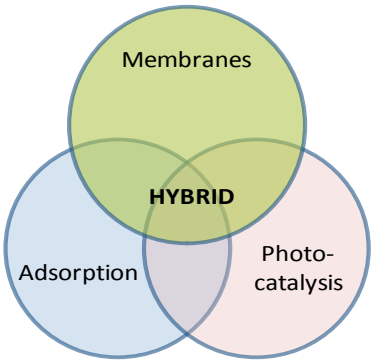


Two different approaches followed to grow zeolites on α-SiC, resulting in; (A) MFI-crystals and (B) ANA-crystals. Schematic representation of the crystal morphology at the SiC interface.

Hybride membrane process for water treatment (HYMEPRO)

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

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



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

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

The objective of the project is to develop a closed process for autotrophic cultivation of microalgae and biorefinery approach using novel extraction techniques for production of algal oils and high-value feed additives from wet algal biomass. The oil will be further converted to biodiesel utilizing a novel immobilized enzymatic technology.

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

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

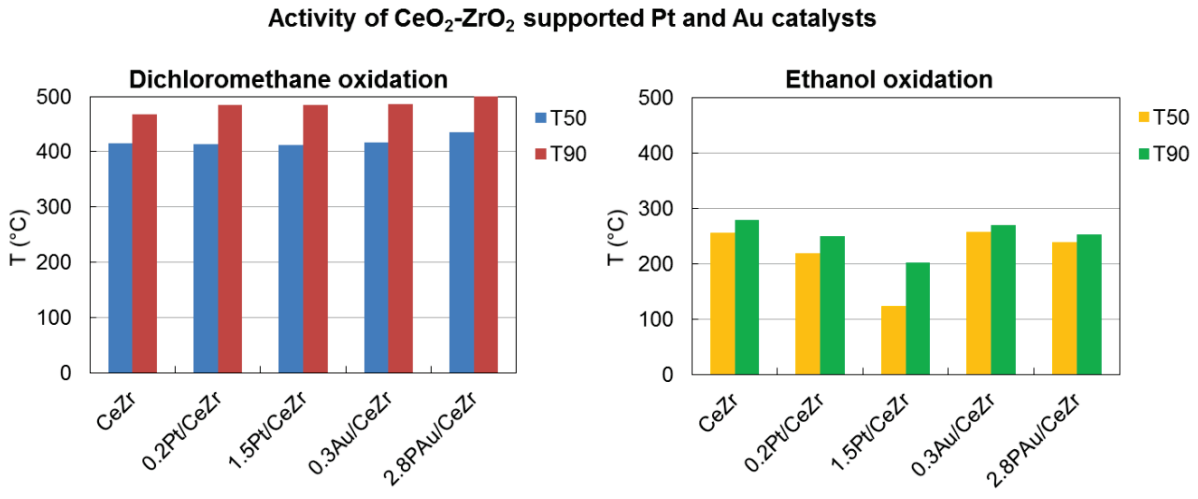
Utilization of vast knowledge of microalgae cultivation techniques and photo-bioreactor existing by partners in Czech Republic will facilitate development of techniques for production of biodiesel feedstock from algal oil. In Israel - TransBiodiesel will contribute to development of non-lipid high tolerance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

Pilot plant bioreactor

Washcoated ceramic monoliths for total oxidation of volatile organic compounds

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

This project is focused on the development of monolithic catalysts for total oxidation of volatile organic compounds based on ceria-zirconia mixed oxide doped by noble metals. Volatile organic compounds are one of the major contributors to air pollution and their emissions are strictly regulated by the directives of European Union. Catalytic oxidation is efficient, cost-effective and environmentally friendly way to treat VOC emissions. In industrial applications, large volumes of gases have to be treated and therefore monolithic catalysts have to be used. Ceramic monoliths are chosen due to their successful application in automotive catalysts and in the industry. The aim of the project is to propose methods for the preparation of highly active and selective monolithic catalysts and to develop the strategy for their tailored synthesis. [Ref. 15]



Activity of ceria-zirconia supported platinum and gold catalysts in the oxidation of dichloromethane and ethanol

International co-operations

Institute of Catalysis, BAS, Sofia, Bulgaria: New heterogeneous catalysts for environmental protection
University of Oulu, Oulu, Finland: New catalysts for VOC oxidation
University of Oulu, Oulu, Finland: Hybrid membrane process for water treatment
University of Paris VI, Paris, France: Theory of chemical bond
University of Poitiers, Poitiers, France: New catalysts for VOC elimination
University of Strasbourg, Strasbourg, France: Determination of transport characteristics of novel materials with hierarchical pore structure
University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
University of Maribor, Maribor, Slovenia: PolyHYPE polymers
University of Graz, Graz, Austria: Porous polymers
Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
University of Barcelona, Barcelona, Spain: Ion exchanger catalysts
Zhejiang University, Hangzhou, China: Mesoporous poly(divinylbenzenes)
Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials
University of Bangor, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials
UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification
University of Udine, Udine, Italy: Characterization of noble metal catalysts and desulfurization on unconventional catalysts
Istanbul Technical University, Istanbul, Turkey: Synthesis and Thorough Characterization of Composite Functionalized Polymeric Nano-Structure
Institute of Computational Chemistry, University of Girona, Spain
IRD Fuel Cells A/S, Svendborg, Denmark: fuel cells electroactivity
Centre National de la Recherche Scientifique, Montpellier, France: non-carbonaceous supports, catalysts
FUMA-TECH Gesellschaft für Funktionelle Membranen und Anlagentechnologie MBH, St Ingbert, Germany: ionomers
Shanghai Jiao Tong University, Shanghai, China: ionomers and polymers
Volvo Technology AB, Göteborg, Sweden: MAE test protocols
SGL Carbon Gmbh, Meitingen, Germany: electroconductive gas diffusive layers
JRC Joint Research Centre-European Commission, Brussels, Belgium: FCH tests
TimCal SA, Bodio, Switzerland: carbon black supports

Visitors

L. Benoit, University of Strasbourg, France
M. Boltz, University of Strasbourg, France
P. Losch, University of Strasbourg, France
P. Krajnc, University of Maribor, Slovenia
J. Grabowski, Central Mining Institute, Katowice, Poland
M. Green, UCG Engineering Ltd, United Kingdom
A. Lobnik, University of Maribor, Maribor, Slovenia
A. Sezai Sarac, Istanbul Technical University Faculty of Sciences

R. Palcheva, Institute of Catalysis, BAS, Sofia, Bulgaria
K. Stanczyk, Central Mining Institute, Katowice, Poland
Y. Zub, Institute of Surface Chemistry NAS, Ukraine
M. Rodlert, TimCal SA, Bodio, Switzerland
F. Mornaghini, TimCal SA, Bodio, Switzerland
G. Tsotridis, JRC Joint Research Centre-European Commission, Brussels, Belgium
I. Galbiati, SGL Carbon Gmbh, Meitingen, Germany
H. Gao, Shanghai Jiao Tong University, Shanghai, China
B. Bauer, FUMA-TECH, St Ingbert, Germany
W. Zhang, FUMA-TECH, St Ingbert, Germany
D. Jones, Centre National de la Recherché Scientifique, Montpellier, France
J. Roziere, Centre National de la Recherché Scientifique, Montpellier, France
J.L. Bonde, IRD Fuel Cells A/S, Svendborg, Denmark
M. Odgaard, IRD Fuel Cells A/S, Svendborg, Denmark
M.J. Larsen, IRD Fuel Cells A/S, Svendborg, Denmark
D.N. Tito, Elysium Projects Ltd., Bangor, United Kingdom

Teaching

P. Klusoň: UJEP, Faculty of the Environment, course "Toxicology"
R. Ponec: CU, Faculty of Science, course "Structure and Reactivity"
O. Šolcová: ICT, Faculty of Chemical Technology, postgraduate course "Texture of Porous Solids"

Publications

Original Papers

[1] Bučinský L., Büchel G.E., Ponec R., Rapta P., Breza M., Kožíšek J., Gall M., Biskupič S., Fronc M., Schiessl K., Cuzan O., Prodius D.: On the Electronic Structure of the mer, trans-[$RuCl_3$(1H-indazole)$_2$ (NO)], a Hypothetical Metabolite of the Antitumor Drug Candidate KP1019: Experimental and DFT Study. *Eur. J. Inorg. Chem.* 14, 2505-2519 (2013).

[2] Centomo P., Bonato I., Hanková L., Holub L., Jeřábek K., Zecca M.: Novel Ion-Exchange Catalysts for Reactions Involving Lipophilic Reagents: Perspectives in the Reaction of Esterifications of Fatty Acids with Methanol. *Top. Catal.* 56(9-10), 611-617 (2013).

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[29] Soukup K., Hejtmánek V., Šolcová O.: Determination of Transport Characteristics of Porous Bio-compatible Materials. In: *Recent Advances in Chemical Engineering, Biochemistry and Computational Chemistry*. (Moller J.A.D., Kibler M.R., Hefferlin R., Ed.), pp. 66-71, WSEAS Press, Athens 2013.

Patents

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Fields of research

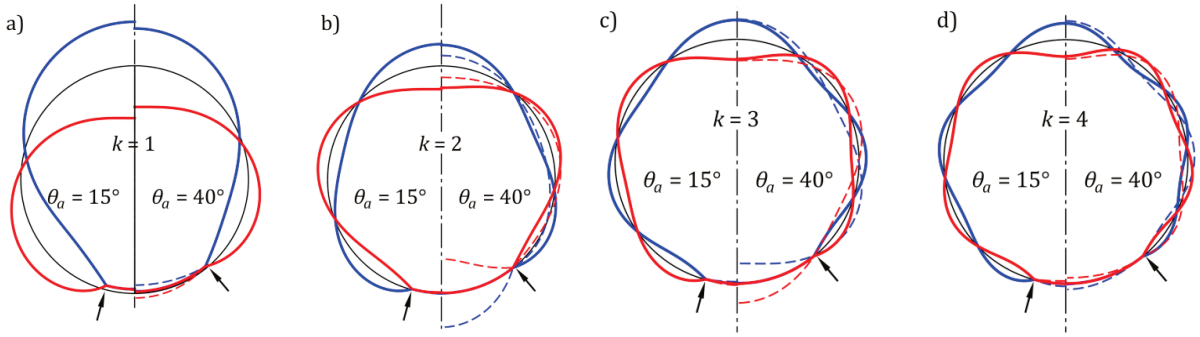
- Multiphase fluid dynamics and transport phenomena in different types of gas-liquid, liquid-solid or gas-liquid-solid systems
- Numerical simulations of transport phenomena in complex multiphase systems
- Influence of surface active agents on the multiphase flows
- Rheometry of microdispersions and non-Newtonian liquids
- Electrodiffusion diagnostics of the flow in microfluidic systems
- Flow characterization in fuel cells
- Hydroacoustic detection of bubbles using sonar in shallow reservoirs
- Sedimentation of polydisperse mixtures and complex ensembles
- Stability and behavior of complex beverage foams

Research projects

Effect of surfactants on the multiphase flow dynamics

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

The effect of surface-active agents on two-phase flows is studied. Flow types "air bubbles in the liquid" and "liquid drops in another immiscible liquid" are focused. Some specific situations, in which the surfactants modify the flow at the bubble/drop scale and in which this modification cannot be explained by a simple change of the equilibrium surface tension, are investigated experimentally. These situations are (i) the shape oscillations of a bubble/drop, both freely-rising or attached at a capillary tip; focus is put on the modification of oscillation frequency and decay time by surfactants; (ii) the coalescence of bubbles/drops, and also their attachment to a solid surface, with a focus on the drainage of liquid film between them; (iii) the bubble-solid surface collision, with a focus on suppression of the bubble rebound caused by surfactants and also on the modification of the attachment time; (iv) break-up of bubbles in a turbulent flow. The research should enlighten and document the effect of interfacial properties other than surface tension on two-phase flows. [Refs. 1, 11-13]

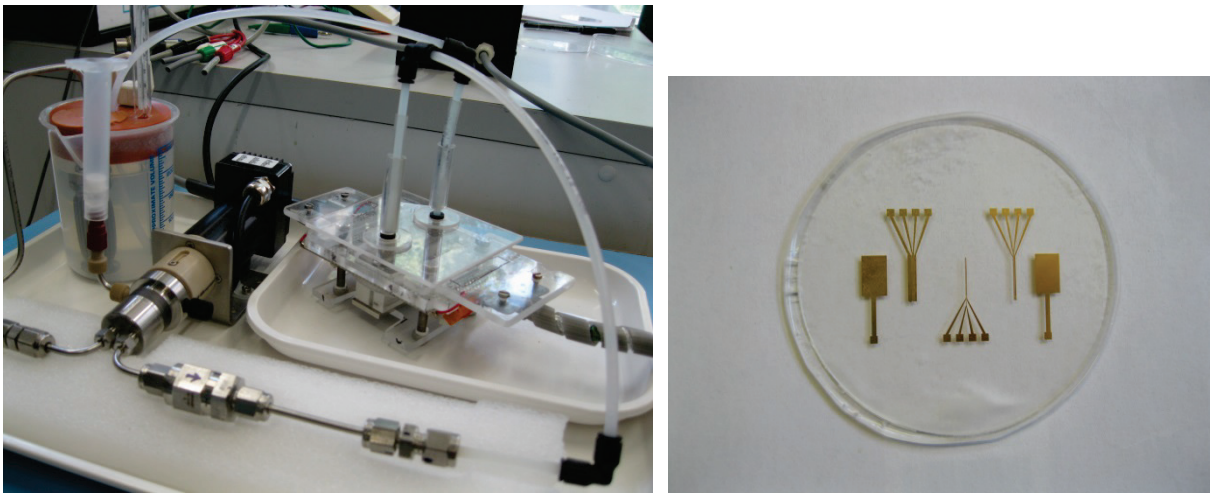


Shape of the first four eigenmodes of a pinned bubble. Left halves of figures represent attachment angle θ=15°, right halves of figures are for θ=40°. The attachment positions are indicated by arrows. Solid lines are for the Strani & Sabbeta constraint, dashed lines are for the Bostwick & Steen constraint.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

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

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

The project is focused on characterization of two-phase flows in microfluidic systems. The high-tech fabrication techniques will be used to produce microdevices with precisely located microelectrodes. These electrodiffusion sensors for the near-wall flow diagnostics will be, for the first time, implemented at a microfluidic scale. The proposed measurements will provide information on the wall shear stress, the local flow structures, and the effect of bubbles/particles on the near-wall flow region (e.g. the liquid film under bubbles, the apparent wall slip in microdispersions). The application of the particle image velocimetry together with the microscopic visualization techniques will complete the hydrodynamic picture of the studied microfluidic flow configurations (junction, crossing, sudden expansion). It is expected that the electrodiffusion method will be proved as a suitable tool for microdevice diagnostics. The obtained experimental knowledge and the derived physical models will be useful for design, control, and optimization of microfluidic devices. [Ref. 9]

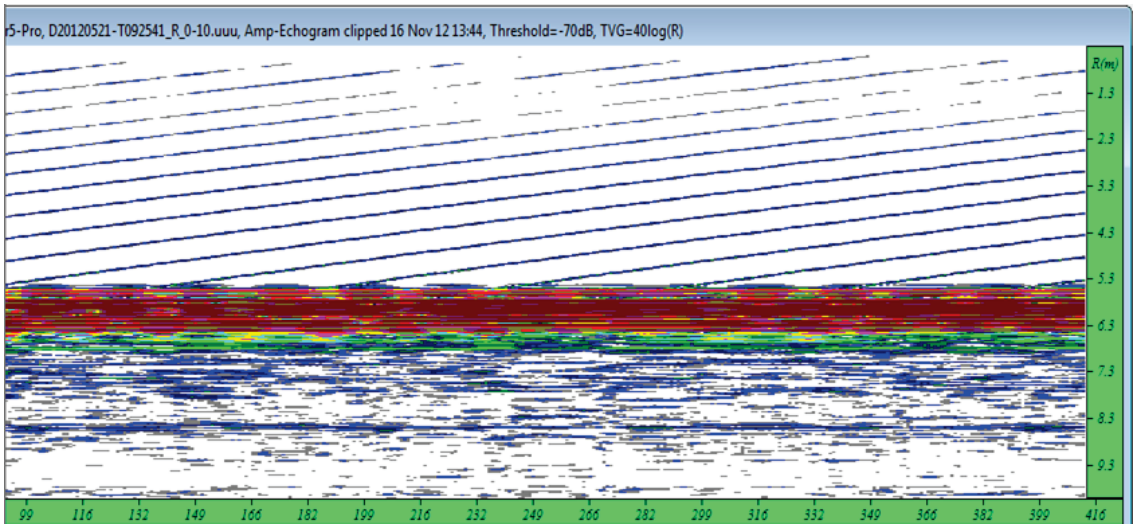


Experimental set-up used for electrodiffusion diagnostics of the flow in microchannels (left) and shown in detail the chip with microsensors (right)

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 ASCR; supported by GA CR, project No. P504/12/1186)

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



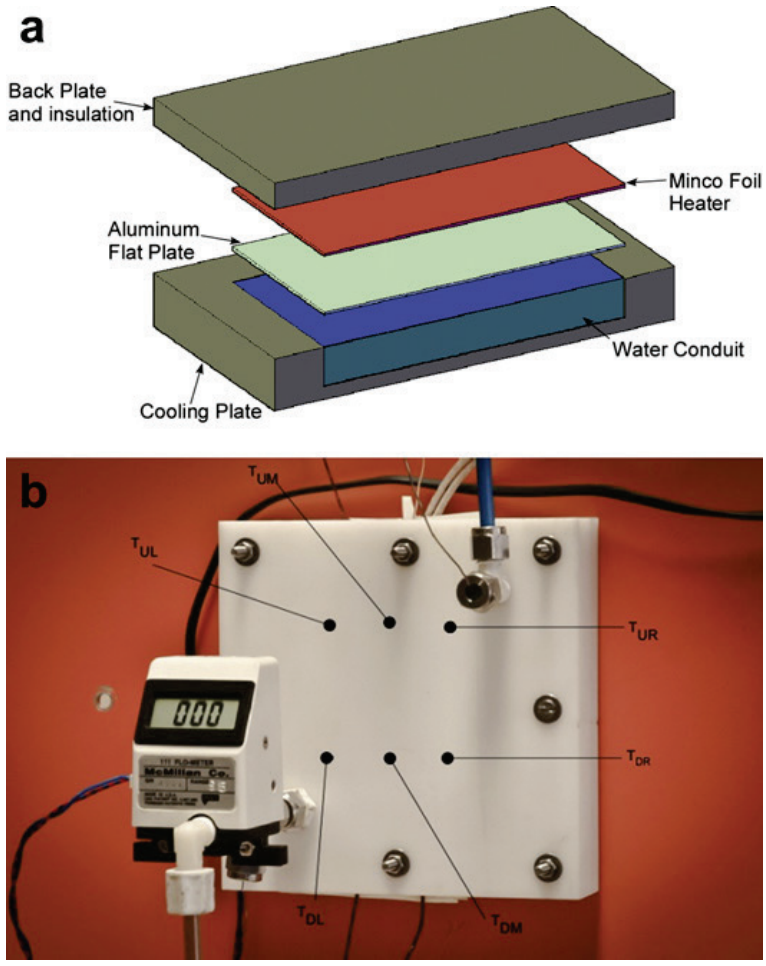
**Acoustic echoes of 3 mm bubbles acquired by vertical 120 kHz sonar.
Blue lines represent rising bubbles and brown bar represents bottom of the lake
(ordinate – water depth, abscissa – time scale in signal pings)**

Optimal heat integration of fuel cell systems

(J. Tihon, tihon@icpf.cas.cz; joint project with Aristotle University of Thessaloniki, Greece; supported by MEYS, project No. 7AMB12GR018)

Objectives of the project are as follows:

1. Develop electrodiffusion microsensors suitable for diagnosing flow in microfluidic devices using photolithography.
2. Use electrodiffusion and micro-PIV (particle image velocimetry) measurement technique to study the structure of the flow in microchannels with complex geometry.
3. Perform CFD (computational fluid dynamics) numerical simulations to study the effect of the geometry of heat exchangers for heat transfer and temperature homogeneity blocks PEM (polymer electrolyte membrane) fuel cells.
4. Propose a methodology for efficient management of heat transfer in mini heat exchangers used to cool the PEM fuel cells.



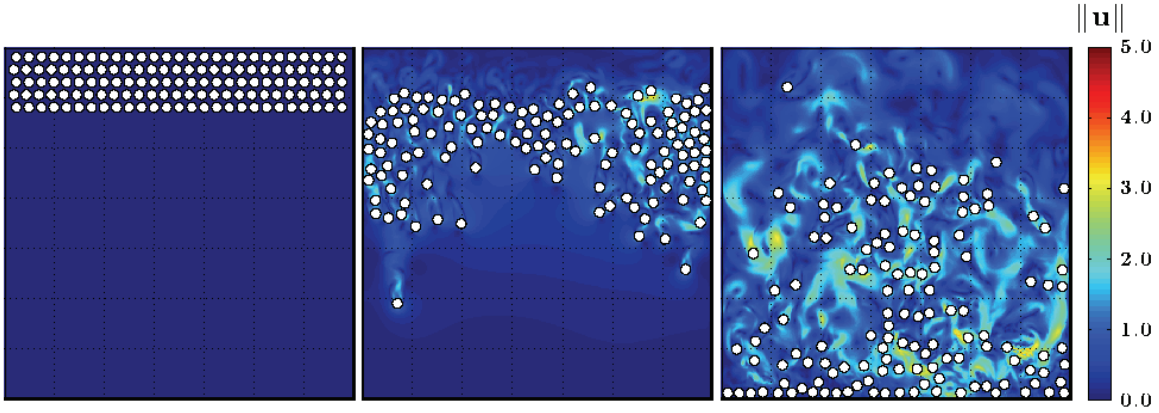
The experimental unit for the study of thermal behavior of the PEM fuel cells in Thessaloniki: (a) schematic representation, (b) photograph with the marked positions of thermocouples

Hydro-mechanical interactions of particles in solid-fluid systems

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

The solid-fluid dispersions are very complicated multiphase systems with a wide range of interactions of different physical nature. The suggested project is focused on specific topic from this field: the hydromechanical interactions between the solid particles (discrete phase)

dispersed in a carrying fluid (continuous phase). The typical feature of these dispersions is the presence of two kinds of force interactions: the fluid forces on the dispersed particles and the mechanical forces between the particles at collisions. These interactions have crucial importance for prediction of flow behavior in process apparatuses or for correct design of industrial technologies. The main aim is to develop physical modeling concepts for solid-fluid dispersions. This concept is based on numerical simulations of these systems and benchmark experiments on static and dynamic behavior. We expect that the project brings important original results, which will help to understand flow behavior of multiphase systems. [Ref. 10]

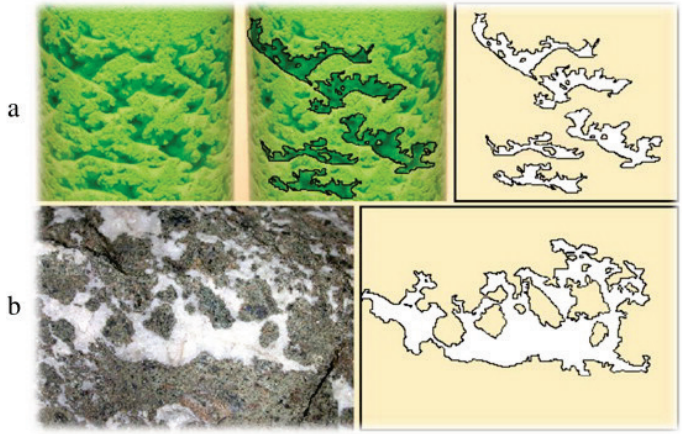


Sedimentation of 135 rigid particles simulated with immersed boundary method

Hydrodynamic concept of stromatactis formation in geology

(M. Růžička, ruzicka@icpf.cas.cz; joint project with Institute of Geology ASCR; supported by GA ASCR, project No. IAAX 00130702)

Stromatactis cavities are present in fine-grained carbonate sediments in nature, forming the specific shapes and reticulate arrays. However, the mechanisms behind the origin of these cavities are subjects of heated discussions in geology for 125 years. Numerous biotic and abiotic factors were considered, but with unclear results. Most recently, our team produced a critical analysis of these sedimentary structures and formulated a new hypothesis that these cavities would likely originate during the rapid deposition of extremely polydisperse and multimodal granular mixtures. Although the first experiments simulated the production of these cavities with a considerably high level of similarity, there is a lot of work to be done if we wish really explain these unique phenomena in terms of hydrodynamics. [Ref. 3]

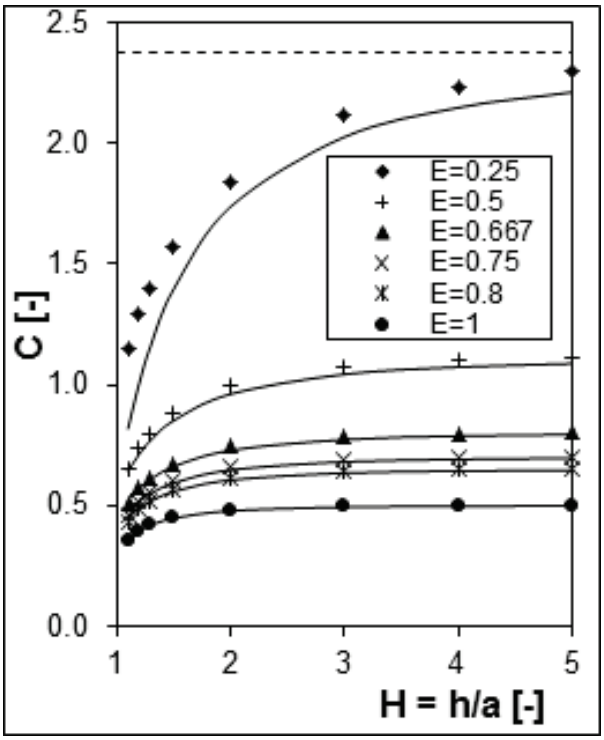


Stromatacta: arching caverns in sedimentary deposits.
a) Artificial man-made laboratory sample (picture width 6 cm)
b) Genuine petrified geological sample (picture width 10 cm)

Added mass closures for multiphase flow systems by means CFD

(M. Šimčík, simcik@icpf.cas.cz)

The added mass coefficient *C* is calculated for dispersed particles in different flow situations using the CFD simulations. Several geometrical configurations are considered, which are physically relevant and difficult to treat analytically. We study a single spherical and ellipsoidal particle near a gas/liquid interface, a pair of ellipsoidal particles in both the in-line and side-by-side arrangements, and an infinite array of spherical particles at different vertical and horizontal spacing. The effect of the key control parameters on the added mass is demonstrated. Where possible, easy-to-use closed formulas (correlations) are provided for the value of *C*. [Ref. 7, 8]



Added mass coefficient *C* for ellipsoidal particle near liquid / gas interface. *C* – particle added mass coefficient, *H* – dimensionless distance of the particle centroid from the interface, h – distance from the interface, a – particle semiaxis (perpendicular to the interface), E – particle semiaxis ratio (a/b)

International co-operations

Centre de Recherché et de Transfert de Technologies, Saint Nazaire, France: Microfluidics
Institute of Fluid Mechanics, Toulouse, France: Effect of surfactants on multiphase flows
Technical University Eindhoven, Eindhoven, The Netherlands: Bubble oscillations
Aristotle University of Thessaloniki, Thessaloniki, Greece: Microfluidics
Norwegian Institute of Technology (NTH), SINTEF, Trondheim, Norway: Bubble columns

Visitors

C. van der Geld, Technical University Eindhoven, The Netherlands
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I. Stogiannis, Aristotle Univ. of Thessaloniki, Greece
T. Sanada, Dept. of Mechanical Engineering, Shizuoka University, Japan
M. I. A. Guerreiro, University of Braga, Braga, Portugal
M. Forest, INP ENSEEIHT Toulouse, France
A. Birem, INP ENSIACET Toulouse, France

Teaching

J. Drahoš, M. Růžička: ICT, Faculty of Chemical Engineering, postgraduate course "Multiphase Reactors"
J. Havlica: UJEP, Faculty of Science, courses "Mathematics", "Chemical Engineering", "Programming in Chemistry", "Numerical Modelling of Heat and Mass Transport"
J. Tihon, J. Vejražka: ICT, Faculty of Chemical Engineering, postgraduate course "Bubbles, Drops, and Particles"
M. Poštůlková: ICT, Faculty of Food and Biochemical Engineering, "Cultivation Techniques and Modeling of Bioprocesses"

Visits abroad

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

Publications

Original papers

[1] Hubička M., Basařová P., Vejražka J.: Collision of a Small Rising Bubble with a Large Falling Particle. *Int. J. Miner. Process*. 121, 21-30 (2013).

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Patents

[14] Brányik T., Růžička M., Poštulková M.: Zařízení pro stanovení přepěňování sycených nápojů. (Czech) Device for determining excessive foam formation of saturated beverages. *Pat. No. 26362*/PUV 2013-28285. Applied: 13.08.05, Patented: 14.01.20.

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Fields of research

- Bioremediation of organic pollutants in soil and sewage
- Immobilization of biocatalysts, living cells or enzymes, into organic or organic-inorganic matrices by sol-gel process
- Whole cell optical sensors
- Application of immobilized biocatalysts in optical sensors
- Dehydrocoupling reactions catalyzed by titanium complexes
- Spin-spin coupling constants $J(^{13}C - ^{13}C)$
- Synthesis of helicene derivatives and [*n*]phenacene derivatives
- Carbosilane metallodendrimers
- Heavy fluorous cyclopentadienes and cyclopentadienyl ligands
- Synthesis of ionic liquids for separation techniques and electrochemical sensing

Applied research

- Enzymatically catalyzed synthesis of alkyd resins
- Development of new analytical methods
- Analytical services to the research departments of ICPF
- Multigram scale production of helicenes and [*n*]phenacenes
- Preparation of helicene based chiral stationary phases for HPLC

Research projects

Measurement of signed carbon-carbon couplings: methods improvements and their application

(V. Blechta, blechta@icpf.cas.cz; supported by ICPF)

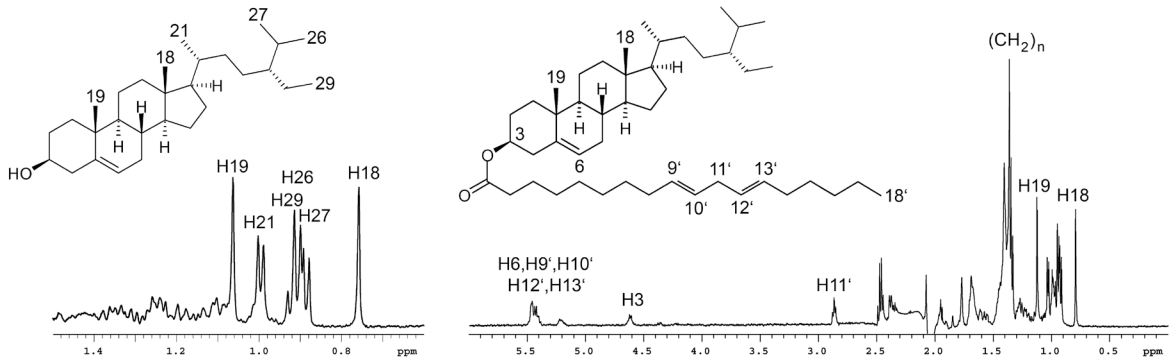
Signed values of all intra-ring $^{2,3,4}J$(C,C) couplings in 9 monosubstituted benzenes (C_6H_5-X where X = F, Cl, Br, CH_3, OCH_3, $Si(CH_3)_3$, C≡N, NO, NO_2) were experimentally determined mainly by new HCSE method as well as 9 couplings to substituent carbons. It was confirmed that while all the vicinal intra-ring ^{3}J(C,C) are positive and all geminal ^{2}J(C2,C4) are negative, both signs are found for geminal ^{2}J(C1,C3) couplings. All the determined signs agree with those already predicted by theoretical calculations.

Performance of HCSE experiment applied to detection of signed carbon-carbon couplings was discussed using a set of already measured samples of 9 monosubstituted benzenes. It was shown that coupling sign detection is insensitive to the settings of carbon-carbon polarization transfer delays. The HCSE spectra of 10 from the total of 43 measured carbon-carbon couplings were considerably influenced by relaxations and proton-proton strong couplings. These effects were quantitatively discussed. The results of HCSE and SLAP experiments were compared. It was shown that the two methods may complement each other in detection of signed carbon-carbon couplings. [Refs. 1, 2]

LC-NMR technique in the analysis of phytosterols in natural extracts

(J. Sýkora, sykora@icpf.cas.cz; supported by ICPF and TACR, project No. TA01010578)

The method shows ability of LC-NMR to detect simultaneously free and conjugated phytosterols in natural extracts. The advantages and disadvantages of a gradient HPLC-NMR method were compared to the fast composition screening using SEC-NMR method. Fractions of free and conjugated phytosterols were isolated and analyzed by isocratic HPLC-NMR methods. The results of qualitative and quantitative analyses were in a good agreement with previously published literature data. [Ref. 3]



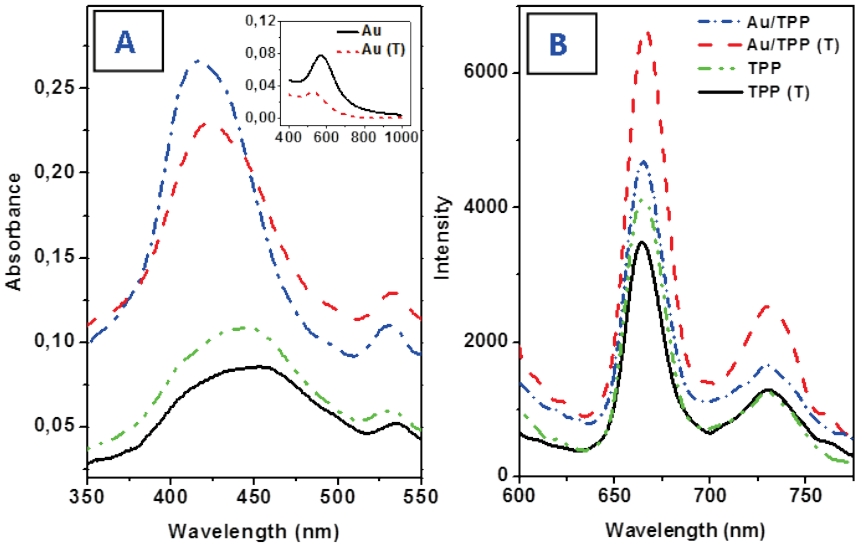
^{1}H NMR spectra of free (left) and conjugated (right) β-sitosterol. Spectra were collected in a stop-flow LC-NMR experiment

Surface morphology and optical properties of porphyrin/Au and Au/porphyrin/Au systems

(A. Solovyev, solovyev@icpf.cas.cz; supported by GACR, project No. 108/11/P840 and 108/12/1168)

Porphyrin/Au and Au/porphyrin/Au systems were prepared by vacuum evaporation and vacuum sputtering onto glass substrate. The surface morphology of as-prepared systems and

those subjected to annealing at 160 °C was studied by optical microscopy, atomic force microscopy, and scanning electron microscopy techniques. Absorption and luminescence spectra of as-prepared and annealed samples were measured. Annealing leads to disintegration of the initially continuous gold layer and formation of gold nanoclusters. An amplification of Soret band magnitude was observed on the Au/meso-tetraphenyl porphyrin (TPP) system in comparison with mere TPP. Additional enhancement of luminescence was observed after the sample annealing. In the case of sandwich Au/porphyrin/Au structure, suppression of one of the two porphyrins' luminescence maxima and sufficient enhancement of the second one were observed. [Ref. 5]



Absorption(A) and luminescence(B) spectra of Au/TPP and TPP films annealed (T) at 1600 °C for 24 h

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

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

Aim of this project is to strengthen education and build up a research team at the FBME (Faculty of Biomedical Engineering) CTU. In the academic year 2012/2013, experiments of three Bc. projects of the students of FBME CTU were realized in the laboratory of Immobilized Biocatalyst and Optical Sensors. The topic of these projects comprised developing XUV radiation sources and their applications in biology and medicine, enzymatic optical sensor, optical fiber biosensor and optical fiber whole-cell sensor of benzene, toluene, xylene and ethyl benzene (BTEX).

Printed Optical Chemical Sensors (POS)

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

We developed a fibre optical sensor of biogenic amines with the enzyme diamine oxidase from *Pisum sativum* immobilized on magnetic carriers (chitosan and acrylate micro beads) with optical oxygen transducer. Application of magnetic carriers enabled substantial simplification of enzyme immobilization. Attenuation of excitation and emission light due to absorption on the dark magnetic microparticles was fully compensated by the electrooptical system. The limits of detection for the biogenic amines putrescine and cadaverine are 25 – 30 μmol L^{-1}, and responses are linear up to a concentration of 1 mmol L^{-1}. [Ref. 8]

Enzymatically catalyzed synthesis of alkyd resins

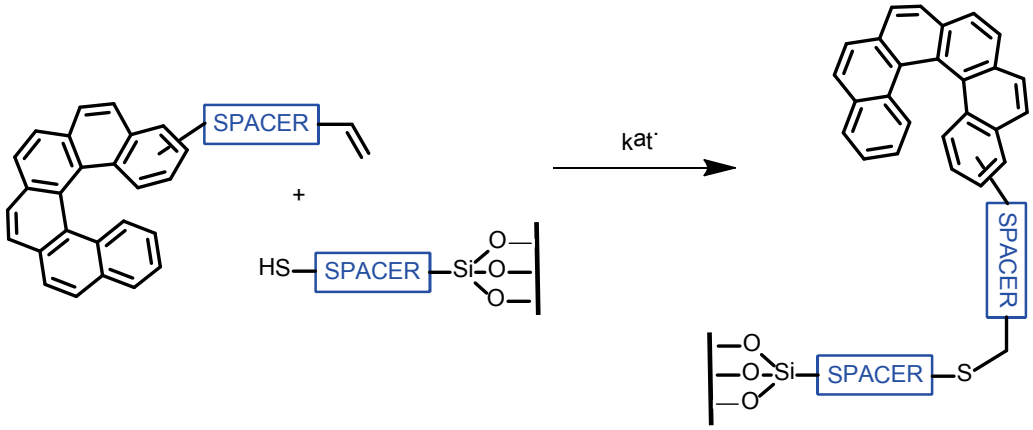
(G. Kuncová, kuncova@icpf.cas.cz; joint project with Synpo, a.s.; supported by MIT, project No. 2A-3TP1/108)

Processes for preparing alkyd resins and/or urethane alkyds and/or urethane oils based on plant and/or animal oils, conducting in two or more steps, lies in enzymatic alcoholysis, at temperature 40 - 70 °C. In the first step plant and/or animal oils and/or fatty acids and/or alkylesters of fatty acids of plant and or animal oils are subjected to transesterification. In the second step alcoholyzates are polycondensated with monocarboxylic and/or polycarboxylic acids and /or monoalcohols and/or polyalcohols. The third step is an addition reaction of alcoholyzate and polycondensate products, in which at first soever isocyanate sequentially monoalcohol are added. In case of preparation of urethane oils the first and third steps of this process are conducted only. [Ref. 15]

Preparation of helicene based chiral stationary phase for HPLC

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

The main aim of the project is to develop a new chiral stationary phase for HPLC which would serve for column manufacturing. The stationary phase is helicene based. The procedure for large scale production of helicene derivatives has been developed and patented. During the third year of project we has explored the 9-bromo[7]helicene reactivity and developed strategy for [7]helicene anchoring. Next step is the enantiomer separation and synthesis of the final chiral stationary phase. Further testing of its properties and evaluation of the relevancy for possible HPLC column production and sale is also part of the project objectives. [Refs. 13, 14]

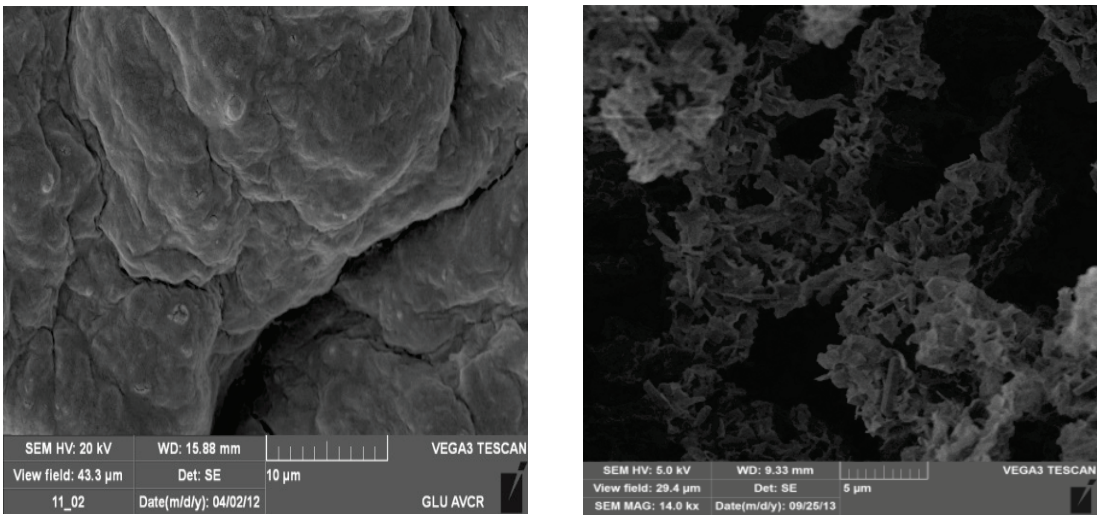


Schematical depiction of the helicene anchoring in order to form stationary phase

Novel inorganic-organic hybrid nanomaterials

(S. Šabata, sabata@icpf.cas.cz; joint project with ICT Prague, IMC, University of West Bohemia Plzeň, supported by ASCR, project No. IAAX08240901)

Na^+ montmorillonite was silanized with methoxy- and ethoxy- organosilanes having various functional groups. The modified montmorillonites were characterized with X-Ray diffraction and used as catalyst carriers. Three types of microbial lipases were adsorbed on the modified montmorillonites. These biocatalysts with adsorbed enzymes were uniaxially frozen in liquid nitrogen (ISISA), dried and characterized with X-Ray diffraction. Activities of newly synthetized nanostructured biocatalysts were compared with commercial one. Esterification of stearic acid with propanol in hexane was chosen as a model reaction. Conversions of stearic acid were 25% in case of lipase – montmorillonite biocatalyst and 92% for biocatalyst frozen in liquid nitrogen.

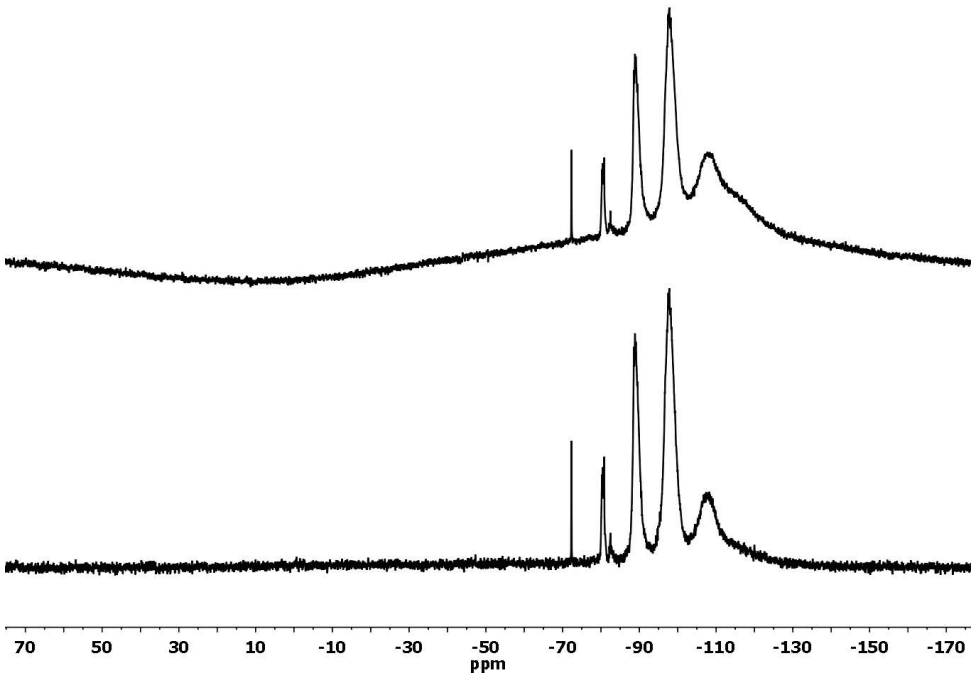


Structure of lipase – montmorillonite biocatalyst (A) - dried at ambient temperature (B) – frozen in liquid nitrogen (ISISA)

Improved Baseline in ^{29}Si NMR Spectra of Water Glasses

(J. Schraml, schraml@icpf.cas.cz; supported by ICPF)

In comparison with traditional NMR measuring methods (top trace) pulse sequence RIDE (bottom trace) eliminates background signal and dramatically improves baseline in ^{29}Si NMR spectra of water glasses. [Ref. 10]



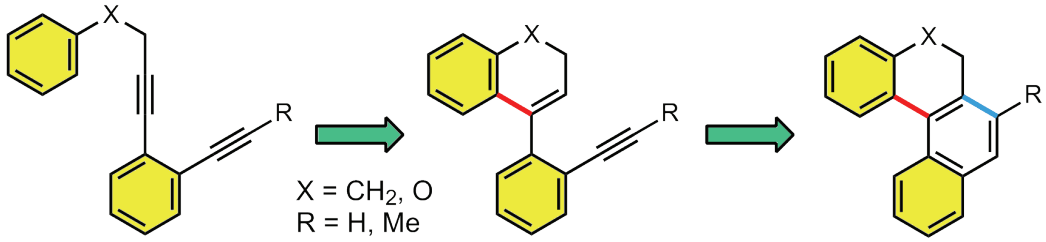
^{29}Si NMR spectra of a sodium water glass measured by one-pulse (top) and RIDE (bottom) pulse sequence

Intramolecular Cascade Hydroarylation/Cycloisomerization Strategy for the Synthesis of Polycyclic Aromatic and Heteroaromatic Systems

(J. Storch, storchj@icpf.cas.cz; supported by TACR, project No. TA01010646)

In the quest of our previous investigations in the field of heterohelicenes for utilization in separation techniques and asymmetric catalysis, we have developed new $PtCl_2/PtCl_4$ catalyzed

hydroarylation/cycloisomerization cascade reaction leading to formation of two aromatic or heteroaromatic rings in one step was reported. The strategy developed is exemplified by the synthesis of 5,6-dihydrobenzo[c]phenanthrene and 6H-naphtho[2,1-c]chromene skeletons. Attempts to [8]helicene-like molecules were also investigated. [Ref. 11]

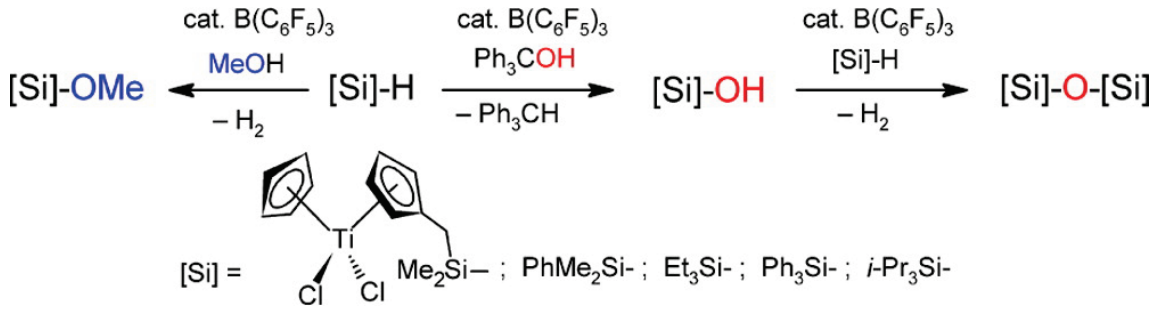


Hydroarylation / cycloisomerization cascade reaction

Reactivity of a Titanocene Pendant Si–H Group toward Alcohols

(T. Strašák, strasak@icpf.cas.cz; joint project with JH IPC; supported by GACR, project No. 203/09/1574 and P207/12/2368).

This work has demonstrated the ability of a novel titanocene dichloride bearing a pendant methylenedimethylsilane group, to achieve methanol silylation in the presence of a catalytic amount of $B(C_6F_5)_3$ in a way similar to that known for commercially available hydrosilanes. A possible extension of the reaction scope to a variety of alcohols could lead to a direct modification of the titanocene periphery with various alkoxo groups in one reaction step. However, Ph_3COH reacted with prepared complex in a different way, and the dimeric titanocene complex with a bis(methylene)tetramethylsiloxane bridge between cyclopentadienyl rings was formed. A detailed study of the $B(C_6F_5)_3$-mediated reaction of Ph_3COH with the model hydrosilane $PhMe_2SiH$ showed that the siloxane formation proceeds in two consecutive steps. The fast initial step consists of hydroxyl group transfer from the trityl moiety to the silicon atom with concomitant formation of the silanol $PhMe_2SiOH$ and Ph_3CH. In the next step, the in situ formed silanol undergoes a $B(C_6F_5)_3$-catalyzed silylation with a second equivalent of hydrosilane to form a siloxane and H_2. The scope of the reaction could be extended to a variety of hydrosilanes. [Ref. 12]



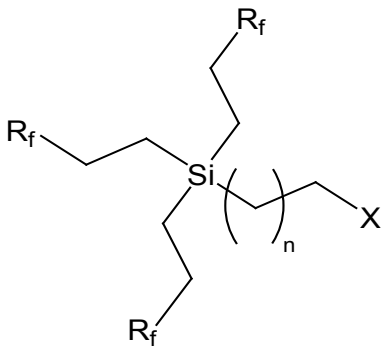
Reactivity of a Si-H group toward alcohols catalyzed by $B(C_6F_5)_3$

Highly fluorous cyclopentadienes for applications in catalysis

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

New approach to the synthesis of heavy fluorous (i.e. showing high fluorophilicity) cyclopentadienes and cyclopentadienyl ligands was studied. The silicon atom is used as a branching atom and three (perfluoroalkyl)ethyl substituents are attached to it. The polyfluorinated synthons of the general formula shown below can be prepared by the reaction of the in situ formed organolithium reagent with silanes $Cl(CH_2)_nSiCl_3$ (n = 2, 3). The X group could

be either halogen (X = Cl, Br, I) or halogen substituent could be replaced by other functional group leading thus to various useful products (X = N_3, C≡CH, C_5H_5). [Ref. 16]



Polyfluorinated synthons and their products; n = 2, 3; $R_f = C_6F_{13}$

International co-operations

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

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

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

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

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

Visitors

S. Ripp, University of Tennessee, USA

Teaching

J. Čermák: UJEP, Faculty of Science, courses "Organic Chemistry I and II", "Chemistry of Heterocyclic and Organometallic Compounds", "Introduction to the Spectral Methods in Organic Chemistry"

G. Kuncová: ICT, Faculty of Chemical Engineering, postgraduate course "Optical Sensors for Measurement in Chemical and Biological Reactors"

Publications

Original papers

[1] Blechta V., Schraml J.: Small Carbon-Carbon Couplings in Monosubstituted Benzenes - Their Signs and Magnitudes Determined by HCSE Method. *Magn. Reson. Chem.* 51(6), 378-381 (2013).

[2] Blechta V., Schraml J.: HCSE Method for Detection of Small Carbo-Carbon Couplings and Their Signs, Comparison with SLAP Pulse Sequence. *Magn. Reson. Chem.* 51(11), 743-749 (2013).

[3] Horník Š., Sajfrtová M., Karban J., Sýkora J., Březinová A., Wimmer Z.: LC-NMR Technique in the Analysis of Phytosterols in Narural Extracts. *J. Anal. Meth. Chem.* 2013, 526818 (2013).

[4] Hudeček O., Budka J., Dvořáková H., Cuřínová P., Císařová I., Lhoták P.: Anion Receptors based on Ureidocalix[4]arenes Immobilised in the Partial cone Conformation. *New J. Chem.* 37(1), 220-227 (2013).

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[6] Mačková M., Himl M., Budka J., Pojarová M., Císařová I., Eigner V., Cuřínová P., Dvořáková H., Lhoták P.: Self-assembly of 5,11,17,23-Tetranitro-25,26,27,28-tetramethoxythiacalix[4]arene with Neutral Molecules and its Use for Anion Recognition. *Tetrahedron* 69(4), 1397-1402 (2013).

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[9] Sajfrtová M., Sovová H., Karban J., Rochová K., Pavela R., Barnet M.: Effect of Separation Method on Chemical Composition and Insecticidal Activity of Lamiaceae Isolates. *Ind. Crop. Prod.* 47, 69-77 (2013).

[10] Schraml J., Sandor P., Korec S., Krump M., Foller B.: Improved Baseline in ^{29}Si NMR Spectra of Water Glasses. *Magn. Reson. Chem.* 51(7), 403-406 (2013).

[11] Storch J., Bernard M., Sýkora J., Karban J., Čermák J.: Intramolecular Cascade Hydroarylation/ Cycloisomerization Strategy for the Synthesis of Polycyclic Aromatic and Heteroaromatic Systems. *Eur. J. Org. Chem.* 2013(2), 260–263 (2013).

[12] Strašák T., Sýkora J., Lamač M., Kubišta J., Horáček M., Gyepes R., Pinkas J.: Reactivity of Titanocene Pendant Si-H Group towards Alcohols. Unexpected Formation of Siloxanes from the Reaction of Hydrosilanes and Ph_3COH Catalyzed by $B(C_6F_5)_3$. *Organometallics* 32(15), 4122−4129 (2013).

[13] Žádný J., Velíšek P., Jakubec M., Sýkora J., Církva V., Storch J.: Exploration of 9-bromo[7]Helicene Reactivity. *Tetrahedron* 69(30), 6213-6218 (2013).

Patents

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[15] Vlček T., Kuncová G., Šabata S., Hetflejš J.: Způsob přípravy alkydových pryskyřic, urethanizovaných alkydů a urethanových olejů. (Czech) Process for Producing Alkyd Resins, Urethane Alkyds and Urethane Oils. *Pat. No. 303842*/PV 2012-147. Applied: 12.03.01, Patented: 13.04.11.

[16] Strašák T., Čermák J.: Polyfluorované činidlo a způsob jeho přípravy. (Czech) Polyfluorinated Reagent and Its Synthesis. *Pat. No. PV 2013-325*. Applied: 13.05.02.

Environmental Process Engineering Laboratory

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Fields of research

- Microwaves in photochemistry and photocatalysis
- Advanced processes for gasification, gas cleaning and hydrogen production
- Persistent organic pollutants and heavy metals emissions and behaviour
- Urban mining - metals recovery from waste ashes
- Fluidized bed gasification of solid, liquid and slurry feedstock
- Medium and high temperature gas cleaning (particularly removal of HCl and H_2S from producer gas) for advanced applications
- Advanced processes for waste-to-energy

Applied research

- Moving bed gasification of wood and waste wood
- Brownfields - Source of renewable energy
- Development and verification of thermal desorption technology using microwaves
- Method for the chemical depolymerization of waste polyethylene terephthalate (PET)
- Complex recycling of compact fluorescent lamps (CFLs) and removal of toxic mercury
- Process for preparing hydrogen by partial oxidation of high-boiling hydrocarbon mixtures and biomass
- Wet precipitators PM for medium-power boilers burning renewable fuels
- Fluidized bed combustion and gasification
- Sewage sludge combustion and co-combustion
- Optimization of waste-to-energy plant and air pollution control devices

Research projects

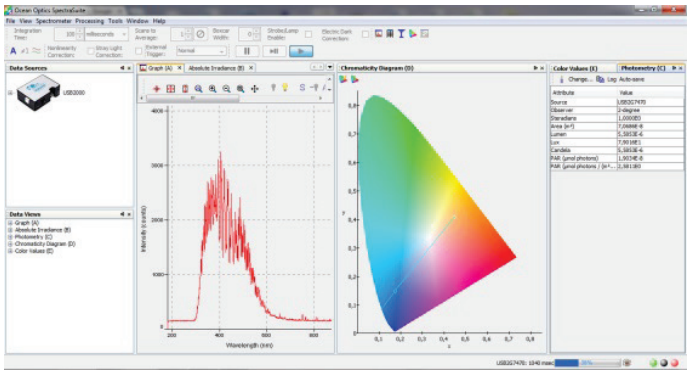
Microwave applications on the field of environmental chemistry, photochemistry and photocatalysis

(V. Církva, cirkva@icpf.cas.cz; supported by ICPF; TACR, project No. TA01010646; and MIT, project No. FR-TI3/628)

The coupled activation of photochemical and photocatalytic reactions by using of two different types of radiation, microwave and UV/Vis, is covered by the new discipline called microwave photochemistry and photocatalysis. Such a connection might have a synergic effect on reaction efficiencies or, at least, enhance them by summing up the individual effects.

The objective of this discipline is frequently, but not necessarily, connected to the electrodeless discharge lamp (EDL) as a novel light source which generates efficiently UV/Vis radiation when placed into a microwave field.

We have applied the concept of microwaves in the field of organic photochemical [9, 12] and photocatalytic synthesis [6], or environmental chemistry [1, 20].

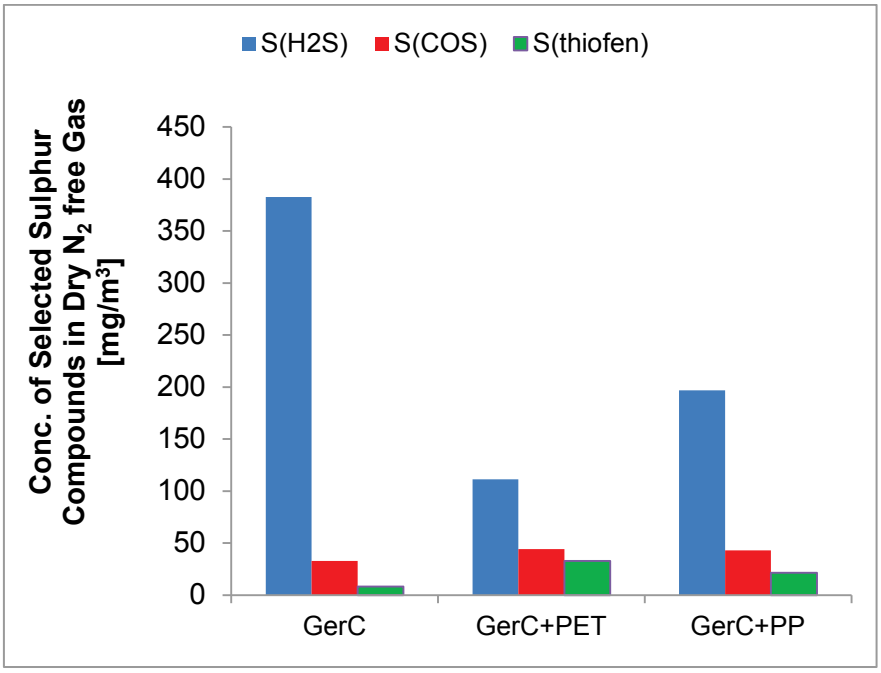


Experimental set-up for microwave photochemical experiments with EDLs

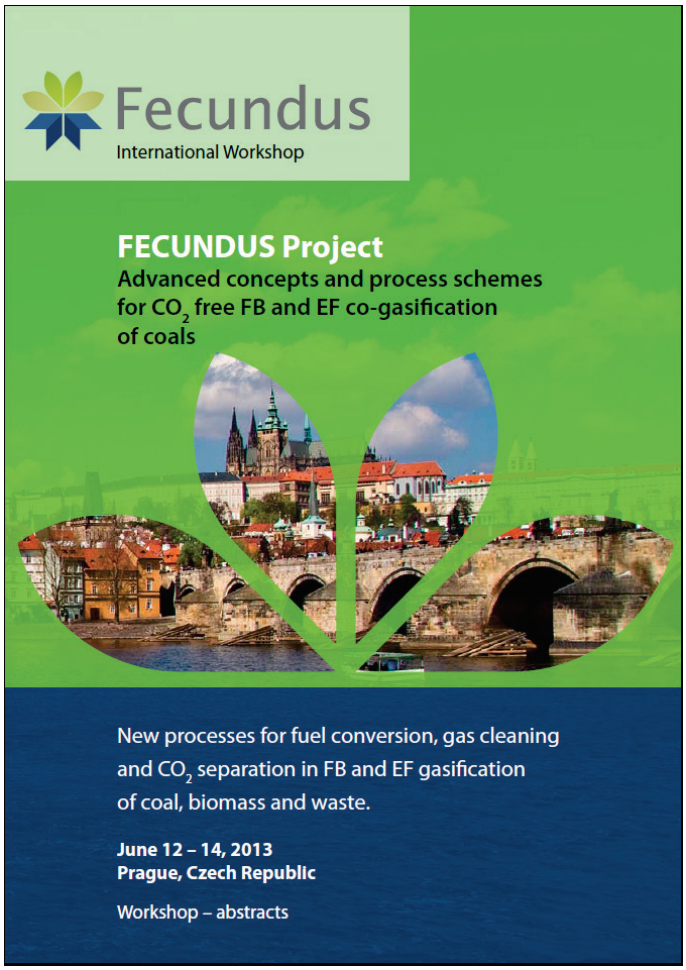
Advanced concepts and process schemes for CO_2 free fluidized and entrained bed co-gasification of coals

(K. Svoboda, svoboda@icpf.cas.cz; joint research project with CNR - Italy, LNEG - Portugal, CIEMAT - Spain, TUV - Austria, ICL - UK, ELCOGAS - Spain, UNISA - Italy; supported by RFCS, project No. RFCR-CT-2010-00009, and MEYS, project No. 7C11009)

The project aims at integrating gasification schemes for the co-gasification of coal, biomass and waste with processes for CO_2 separation and capture. Fluidized bed and entrained flow gasification processes are considered thanks to their flexibility and effectiveness for carrying out thermal conversion of different feedstock, for matching different requirements of producer gas end-users and for effective CO_2 separation. Fuel feeding in a form of solid particles, mixtures of solid particles and various slurries (suspensions of solid fuel particles) and different fluidized bed particulate materials (sand, dolomite, olivine) are compared in terms of their effects in fluidized bed gasification. Effects of both, primary measures (involved in overall conditions of a given gasification process) and secondary (downstream) measures on syngas properties (particularly composition, purity and heating value) and possible applications are studied as well as effects of partial substitution of steam by CO_2 in gasification medium on gasification characteristics and producer gas properties. At the end of the project solution period (June 12-14, 2013) the international workshop on *"New processes for fuel conversion gas cleaning and CO_2 separation in FB and EF gasification of coal, biomass and waste"* was organized in Prague. Invited lectures of foreign experts have been presented. [Refs. 2, 4, 5, 11, 15, 16]



Comparison of concentrations of selected sulfur compounds (H_2S, COS and thiophene) in dry, N_2-free producer gas for fluidized bed (FB) gasification of German coal with gas concentrations of the sulfur compounds in FB co-gasification with PET (24 wt. %) and PP (20 wt. %). T = 850 °C, air/steam, ER = 0.21, H_2O/C mol. ratio ≈ 1, FB-material: sand/dolomite ≈ 1/1

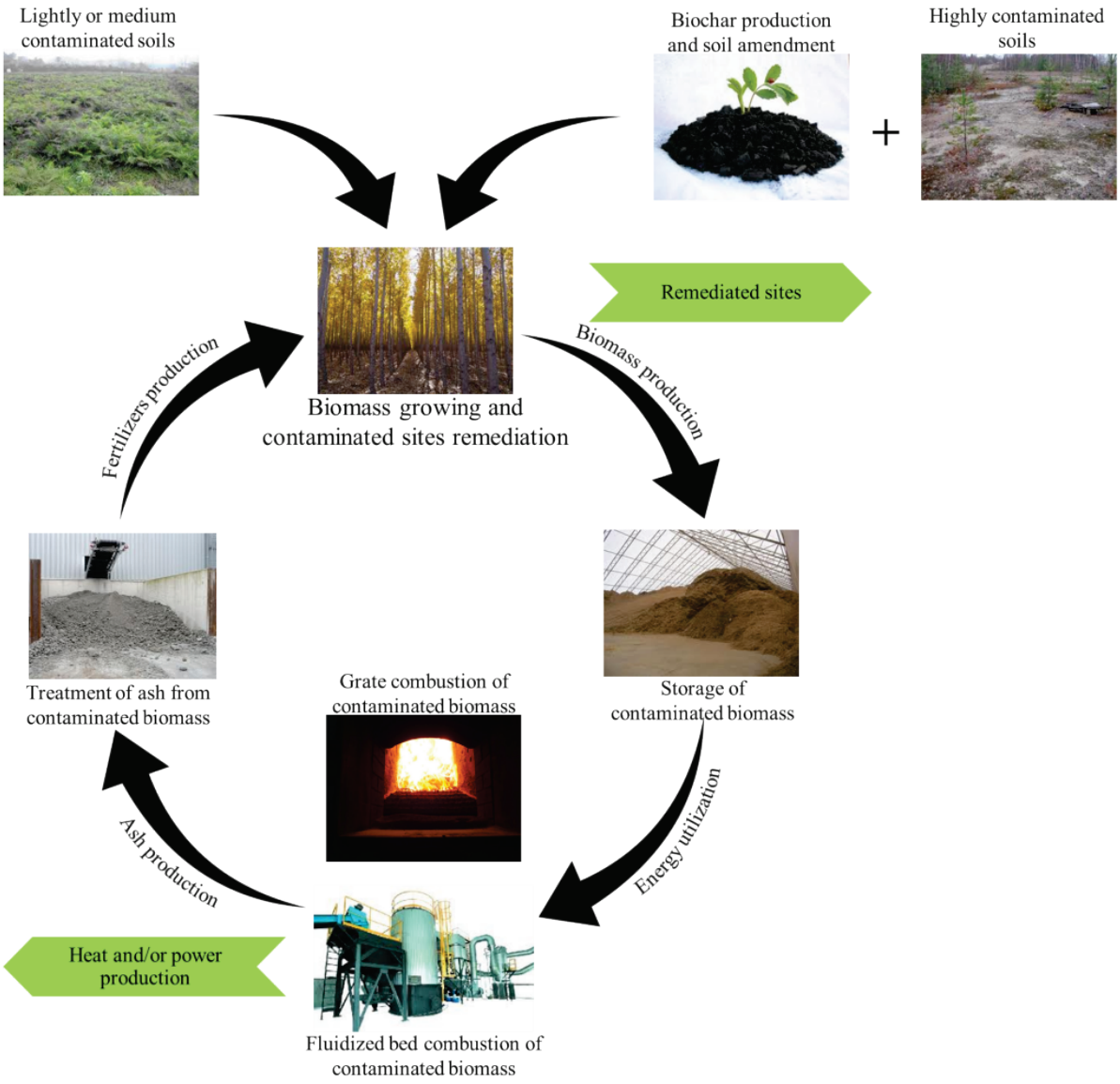


Front page of the Proceedings from the International workshop of the Fecundus project

Brownfields - Source of renewable energy

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

The phytoextraction ability of some fast-growing plant species leads to the idea of connecting biomass production with soil remediation on contaminated industrial zones and regions. This biomass will contain significant amount of heavy metals and its energetic utilization has to be considered carefully to minimize negative environmental impacts. Therefore, the behavior of selected heavy metals was observed during thermal treatment of contaminated biomass. Moreover, a detailed analysis of trace and nutrient elements distribution and chemical speciation in ashes was performed. The potential of the application of these ashes and methods of treatment for heavy metals removal was evaluated. This knowledge is essential for further utilization of all products of gasification and for the fulfillment of emission limits during combustion. The concept of contaminated biomass growing and utilization was proposed. [Refs. 11, 15, 16]



The concept of contaminated biomass growing and utilization

Development and verification of thermal desorption technology using microwave radiation

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

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

In this study, were compared efficiencies of persistent organic pollutants (POPs) removal from solid materials (soil and building waste) using conventional and microwave heating. These experiments were performed in laboratory apparatus and pilot scale devices. It was confirmed that more polar pollutants (for example chlorinated pesticides) can be effectively

removed at a temperature below their boiling point. Probably, this effect was evoked through co-transport some contaminants with water vapour. Microwave heating was a very applicable alternative heating method that brings about faster heating of the material and saving of energy. The examined groups of pollutants (pesticides and PCBs,) were removed with high efficiency at temperatures around 250 °C. [Refs. 7, 21]

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

Advanced method using microwaves for repair of damaged roads

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

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

The quality tests of repaired place showed that after 3 years good quality of repaired place by microwave heating was obtained. Present research is now focused on reparation of roads with low absorption for microwaves. [Ref. 13]

Progressive method and new equipment using microwaves for drying of surfactants

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

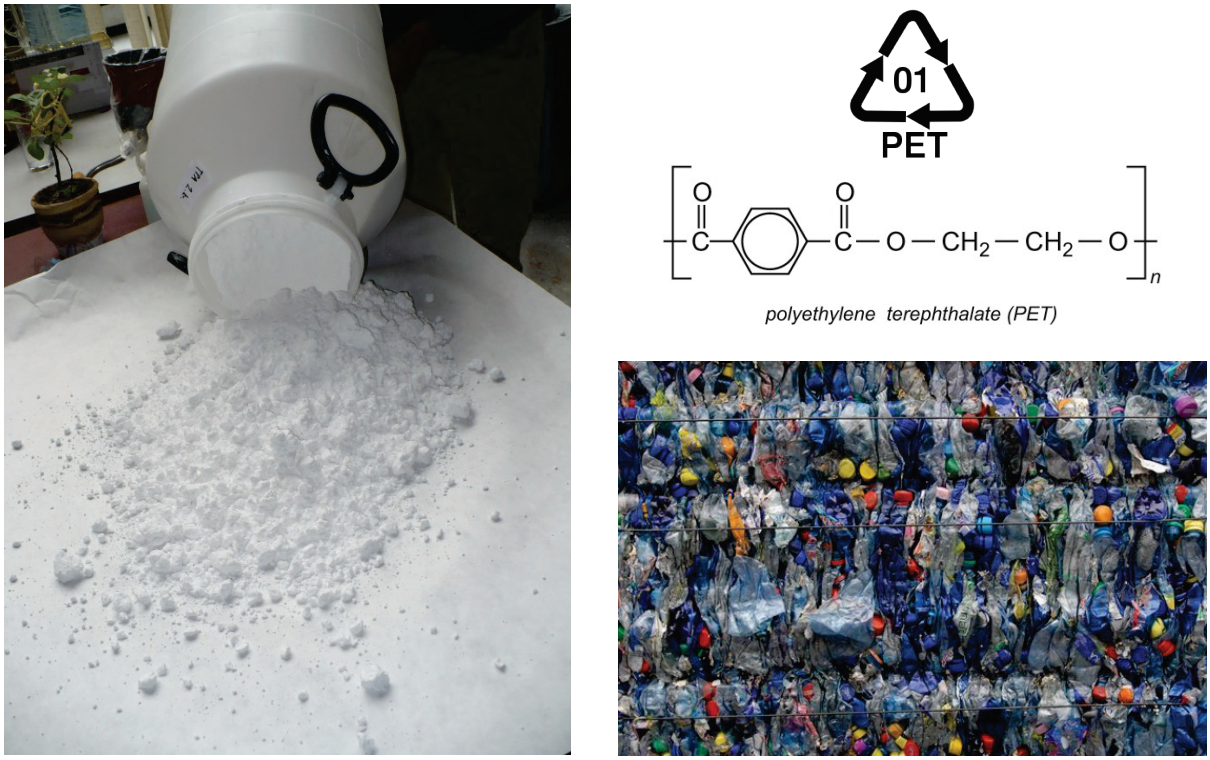
The method and equipment making use of microwaves was applied on drying of surfactants from water solutions. It was found that use of microwave heating provides better quality of dried surfactants compared to conventional method. Drying was performed under mild condition and was found that process was significantly energy saving. The aim was to prepare such different surfactants (anion-active, cation-active, non-ionic, and/or amphoteric) in powder form having a high quality. [Refs. 14, 19]

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

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

The recycling of waste PET is currently one of the most important tasks in the polymers recycling industry. In ICPF, the unique technology for processing of waste PET material on appropriate monomers (i.e. terephthalic acid and ethylene glycol) was developed. This new method for the chemical depolymerization of PET by application of microwaves was applied. One advantage of this method over others is that it does not require sorting before processing.

The mentioned method is patented in Czech Republic (patent No. CZ299908) and also in foreign countries (patent No. EP2176327, WO2009010435, and CN101688015). Successful technology was verified on microwave reactor with working capacity of 280-1000 L. In 2013 was started in Poland the construction of factory with capacity of 10 000 ton of PET per year. The realization of microwave technology is supported by the European Union.



Purified terephthalic acid, chemical formula of PET, and waste PET bottles

Complex recycling of compact fluorescent lamps (CFLs) and removal of toxic mercury contained in input material

(V. Gruber, A. Heyberger, gruber@icpf.cas.cz, heyberger@icpf.cas.cz; joint project with Recyklace Ekovuk, a.s., supported by TACR, project No. TA02021290)

Project was solving the new complex recycling method of compact fluorescent lamps (CFLs) with mercury content: from controlled destruction over the part sorting on glass, metal and luminophore, separation of mercury from luminophore and mercury conversion to chemical stable form suitable for deposition or repeated utilization, up to isolation of precious components (yttrium and europium) and their repeated utilization at fabrication of lighting devices. Pilot plant unit was constructed in cooperation with Kwa-Zulu Natal University, Durban, Republic of South Africa, and is just being prepared to start the operation. [Ref. 18]

Apparatus for recovery of rare metals

Process for preparing hydrogen by partial oxidation of high-boiling hydrocarbon mixtures and biomass and apparatus for making the same

(V. Veselý, J. Hanika, vesely@icpf.cas.cz, hanika@icpf.cas.cz; joint project with VÚAnCh, a.s., Ústí n. Labem and ICT; supported by MIT, project No. MPO 2A-2TP1/024)

The present invention relates to a process for preparing hydrogen by partial oxidation of high-boiling hydrocarbon mixtures and biomass wherein the invented preparation process is characterized in that biomass with moisture level of 10 % at the most is treated to a particle size in the range of 0.1 to 0.5 mm. Subsequently, so treated biomass is then mixed in a high-boiling hydrocarbon mixture. The biomass and the high-boiling hydrocarbon mixture ratio ranges within 4:100 to 12:100. Finally, an oxygen-steam mixture is added. The reaction mixture reacts within a reactor at a temperature ranging from 1100 to 1250°C, at a pressure in the range of 3 to 4 MPa and with a dwell of 7 to 20 s to obtain hydrogen and synthesis gases. In the invention, there is further described an apparatus for making the above-indicated preparation process. [Refs. 3, 8]

Quench of the POX reactor

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

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

Project is developed the new technology for separating solid particles from flowing mass of air, especially for middle-burning source of renewable biomass resources and the technology present in the form of a utility model and a prototype of representative size. The size of the prototype was chosen to allow transfer of results of experimental research and development in commercial use after project completion. [Ref. 8]

Wet separator for flying ash

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

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

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

International co-operations

Central Mechanical Engineering Research Institute, Durgapur, India: Waste gasification

Institute for Energy and Transport, Joint Research Centre of EC, Petten, the Netherlands: Atmospheric and pressurized fluidized bed combustion/gasification technologies; Waste incineration/gasification

University of KwaZulu-Natal, Durban, Republic of South Africa: Gaseous and particulate emissions

The Vienna University of Technology, Austria: Fluidized bed biomass gasification

Imperial College, London, United Kingdom: Pressurized FB gasification, combination with SOFC

The Combustion Research Institute, National Research Council, Napoli, Italy: In-bed catalytical processes for fluidized bed gasification and tar reduction

Institute of Nuclear Energy Research, Atomic Energy Council, Taiwan: Development of fluidized bed gasification with efficient gas cleaning, chemical looping production of hydrogen

Laboratório Nacional de Energia e Geologia, Portugal: Syngas cleaning, removal of tar, sulfur and nitrogen compounds

Visits Abroad

P. Kameníková: Hawaii Natural Energy Institute, University of Hawaii, USA (6 months)

Visitors

M. Čársky, University of Kwazulu-Natal, Durban, Republic of South Africa

Y.-P. Chyou, Institute of Nuclear Energy Research (INER), Taiwan

Teaching

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

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Original papers

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[2] Elsasser T., Pohořelý M., Jecha D., Punčochář M., Stehlík P.: Thermische Klärschlammbehandlung in der Tschechischen Republik und experimentelle Bestimmung der Emissionen aus der Verbrennung. *Chemie Ingenieur Technik* 85(12), 1-7 (2013).

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[5] Hartman M., Svoboda K., Pohořelý M., Šyc M., Jeremiáš M.: Attrition of Dolomitic Lime in a Fluidized-Bed at High Temperature. *Chem. Pap.* 67(2), 164-172 (2013).

[6] Kmentová H., Církva V.: Microwave Photocatalysis IV: Effects of Additional Operational Parameters on the Microwave Photocatalytic Degradation of Mono-Chloroacetic Acid Using Titania-Coated Mercury Electrodeless Discharge Lamps. *J. Chem. Technol. Biotechnol.* 88(6), 1109-1113 (2013).

[7] Mašín P., Hendrych J., Kroužek J., Kubal M., Kochánková L., Sobek J.: Removal of Persistent Organic Pollutants from a Solid Matrix by Thermal Desorption Technology Using Conventional and Microwave Heating. *Fresenius Environ. Bull.* 22(7A), 2017-2021 (2013).

[8] Veselý V., Hanika J., Tukač V., Lederer J., Kovač D.: Catalytic Partial Oxidation of Biomass/Oil Mixture. *Journal of Energy and Power Engineering* 7(10), 1940-1945 (2013).

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Review papers

[10] Punčochář M.: Institute of Chemical Process Fundamentals of the ASCR: Expectation. *Kemija u industriji* 62(5-6), 214-215 (2013).

Patents

[11] Pohořelý M., Kameníková P., Svoboda K., Skoblia S., Jeremiáš M., Šyc M., Punčochář M., Hartman M.: Zařízení pro fluidní zplyňování tuhých paliv. (Czech) The Facility for the Fluidized-Bed Gasification of Solid Fuels. *Pat. No. 304060*/PV 2012-516. Applied: 12.07.27, Patented: 13.07.31.

[12] Storch J., Církva V., Bernard M., Vokál J.: Způsob výroby [6]helicenů fotocyklizací. (Czech) Method and Apparatus for Production of [6]Helicenes. *Pat. No. 303997*/PV 2012 - 245. Applied: 12.04.11, Patented: 13.06.26.

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[19] Sobek J., Hájek M., Práda D., Ba A., Bartůněk P.: Zařízení pro sušení tenzidů. (Czech) Equipment for Drying of Surfactants. *Pat. No. 26524*/ PUV 2013-27960. Applied: 13.05.22. Patented: 14.03.12.

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Department of Aerosols and Laser Studies

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LAB TECHNICIANS
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Fields of research

- Atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- Synthesis of nanoparticles *via* aerosol processes
- Heat and mass transfer in aerosol systems
- Interaction of aerosols with electromagnetic radiation
- Emissions sampling
- Nanoparticles and health
- Aerosol technology
- IR and UV laser induced chemistry
- Chemical vapor deposition of novel C-, Si- and Ge-based nanostructured materials
- IR laser-induced carbothermal reduction of oxides
- UV laser deposition of SERS active substrates based on Ag/graphene
- CVD of nanostructured objects (nanowires, nanoplatelets)
- IR and UV laser deposition of Ti/O-based materials
- IR and UV laser ablation for deposition of thin films, multilayers and nanocomposites

Research projects

Human EXposure to Aerosol COntaminants in Modern Microenvironments

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

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

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

Aerosols, Clouds, and Trace gases Research Infra Structure Network

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

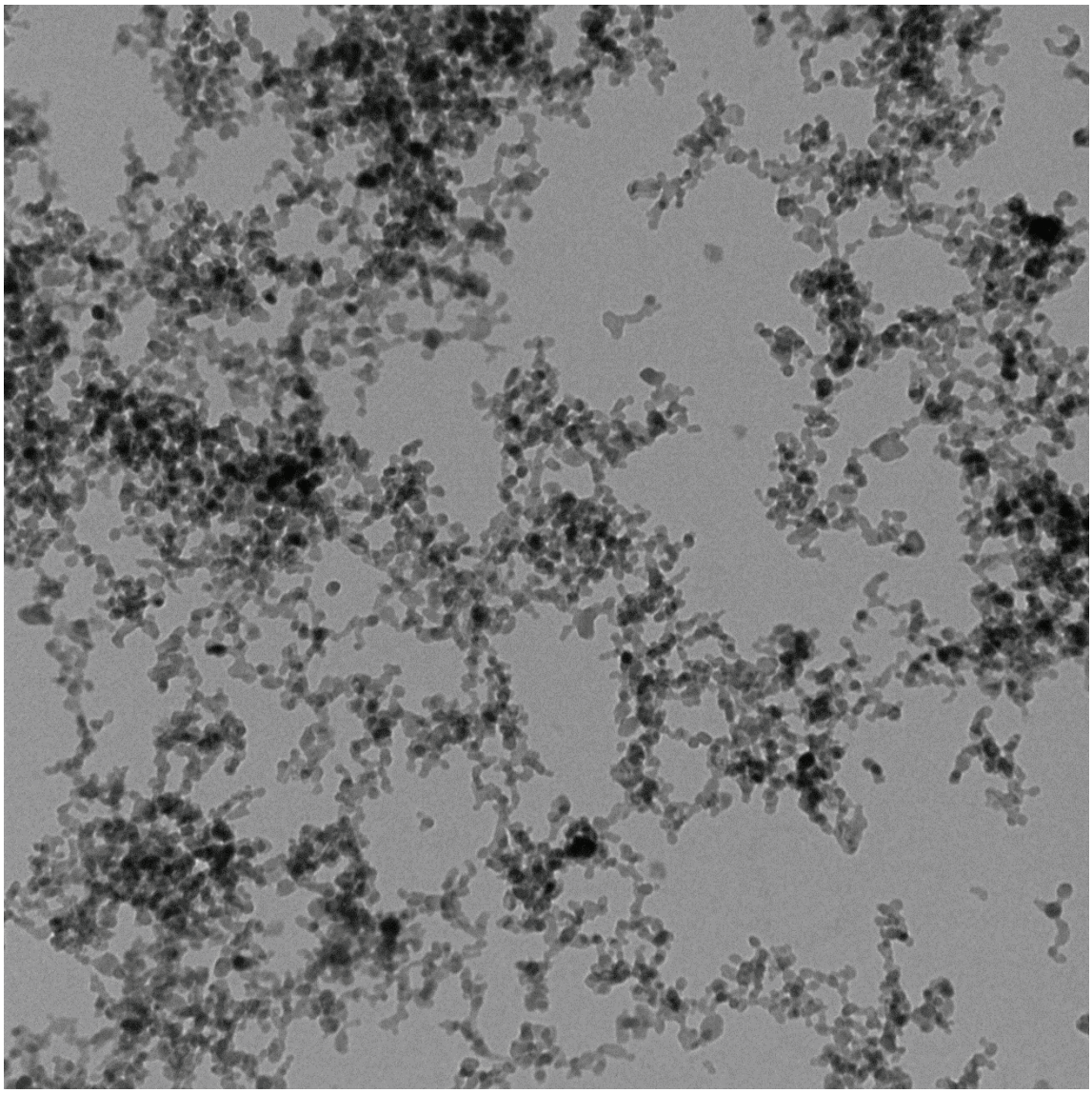
ACTRIS (Aerosols, Clouds, and Trace gases Research Infra Structure Network) is an European Project aiming at integrating European ground-based stations equipped with advanced atmospheric probing instrumentation for aerosols, clouds, and short-lived gas-phase species. ACTRIS will have the essential role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

ACTRIS is building the next generation of the ground-based component of the EU observing system by integrating three existing research infrastructures: EUSAAR, EARLINET, CLOUDNET, and a new trace gas network component into a single coordinated framework. ACTRIS is funded within the EC FP7 under "Research Infrastructures for Atmospheric Research". [Refs. 1, 13]

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.



TEM image of TiO_2 (anatase) nanoparticles generated for inhalation experiments by thermal decomposition of titanium tetra-isopropoxide at T_R=900 °C, Q_R=1200 cm^3/min, P_{TTIP}=1.9 Pa, image area 1.36x1.36 µm. Notice quite uniform nanoparticles with typical size 12 – 20 nm

Thermophysical properties of water in unexplored, technologically significant regions

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

This project focuses primarily on liquid water and solutions of selected salts below the freezing point (supercooled water), and water in nano-droplets. Existing hypotheses include the possibility of phase separation of supercooled water into two liquid phases below the second critical point. Density of supercooled water is only known at 0.1 MPa. Suggested measurements up to 100 MPa will provide first data. A new method and apparatus will be developed. The surface tension of supercooled water and a salt solution will be measured. The surface tension of nano-droplets will be estimated from nucleation experiments. A range of theoretical approaches including phenomenological methods, simplified microscopic models, and molecular simulations, will be used with experimental data to obtain fundamental findings and engineering models. [Refs. 11, 12, 17, 18, 22, 23]

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

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

Advanced physical and chemical properties of Central European atmospheric aerosol at rural background and urban background sites will be studied in high time and size resolution. Parallel measurement of aerosol volatility will be carried out using a C-ToF-AMS equipped with a thermodenuder inlet, aerosol hygroscopicity using an Hygroscopic Tandem Differential Mobility Analyser (HTDMA), and particle number size distribution using an Scanning Mobility Particle Sizer (SMPS). The information about aerosol particle density will be extracted from the SMPS and AMS. Hygroscopicity closure will be obtained from the combined HTDMA and AMS chemical composition data allowing to study the influence of organic aerosol on particles' hygroscopicity. The content of primary and secondary organic aerosol and the extent of aerosol ageing will be determined using AMS data at each site. In addition, at least a year-long time evolution of number size distributions obtained using the SMPS and OC/EC concentrations from the OC/EC analyzer will be delivered to the EBAS database, to be available for global atmospheric modeling groups. [Refs. 19, 21]

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

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

The aim of the project is to determine some properties of heterogeneous nuclei present in the superheated steam of steam turbines. In this project, the sampling device, coupled to advanced aerosol instrumentation (condensation particle counter, scanning mobility particle sizer), will be used to measure heterogeneous particles at selected power stations. To enable measurements of particles down to about 1 nm, a fast expansion chamber will be developed, enabling resolution of particle size by variable supersaturation. Collected data will serve as a basis for understanding the transport and the state of agglomeration of chemicals present in the steam circuit, for quantifying their effect on condensation, and, consequently, on the efficiency and reliability of steam turbines. [Ref. 8]

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

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

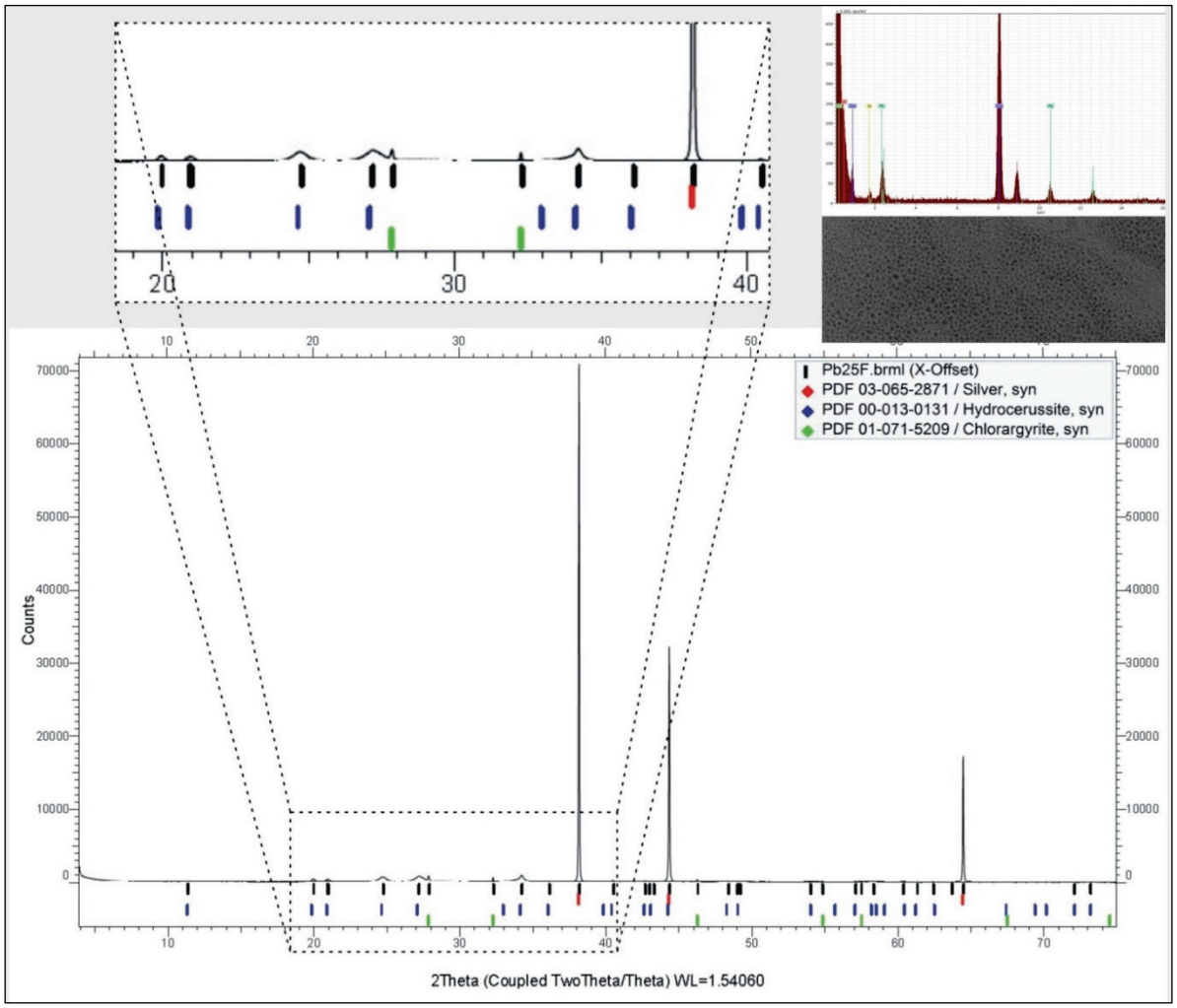
The method intercomparison studies will be conducted both under summer and winter conditions at both sites lasting 2 weeks each. By pooling the instruments and expertise of the two partners, BC will be measured on-line with the MAAP and the aethalometer techniques and from filter samples with the integrating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

Study of transport of inhaled nano-sized particles (Pb, Cd) and their allocation in organs

(J. Smolík, smolik@icpf.cas.cz; supported by GACR, project No. 503/11/2315)

All of the evidence from animal and human studies showed that there are risks associated with inhalation of nano-sized particles (NSP). The alveolar translocation of NSP is likely the pathway how NSP can be transposed from air to the blood vessels, and distributed throughout

the body to organs. In spite of the fact that an extrapulmonary translocation is highly dependent on particle surface characteristics/chemistry, in addition to particle size, the study of transport of inhalated nano-particles Pb, Cd (elements, oxides), their allocations in organs, as well as study of toxicity these nanoparticles will be carry out with nanoparticles (10, 20 and 60 nm). The nonbiogenous elements (Cd, Pb) have been selected as products of technological processes and due to their presence in ambient aerosol. The research will give us more information for a proper understanding of risks of technologies producing Cd and Pb nano-sized particles and ambient aerosol risk.



XRD spectrum and TEM image with EDS spectrum (inset) of Pb nanoparticles generated by PVD method. Notice the effect of atmosphere (O_2, CO_2 and humidity) during two weeks between synthesis and XRD analysis on the change of composition from Pb to hydrocerussite [$Pb_3(CO_3)_2(OH)_2$]

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

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

The aims of the project are: a) development of evaluation methods for indoor air quality in libraries and archives, targeted at reduction of damages on library and archival collections caused by adverse effects of environment and b) gaining detailed knowledge of direct dependences between damage of library and archival collections and surrounding environment, leading to precautions reducing the adverse effects of deteriorated environment. [Refs. 14, 16]

Particle number concentrations measured at library of Regional Museum at Teplice

Preparation of thin layers of ferromagnetic semiconductors

(R. Fajgar, fajgar@icpf.cas.cz; supported by ICPF)

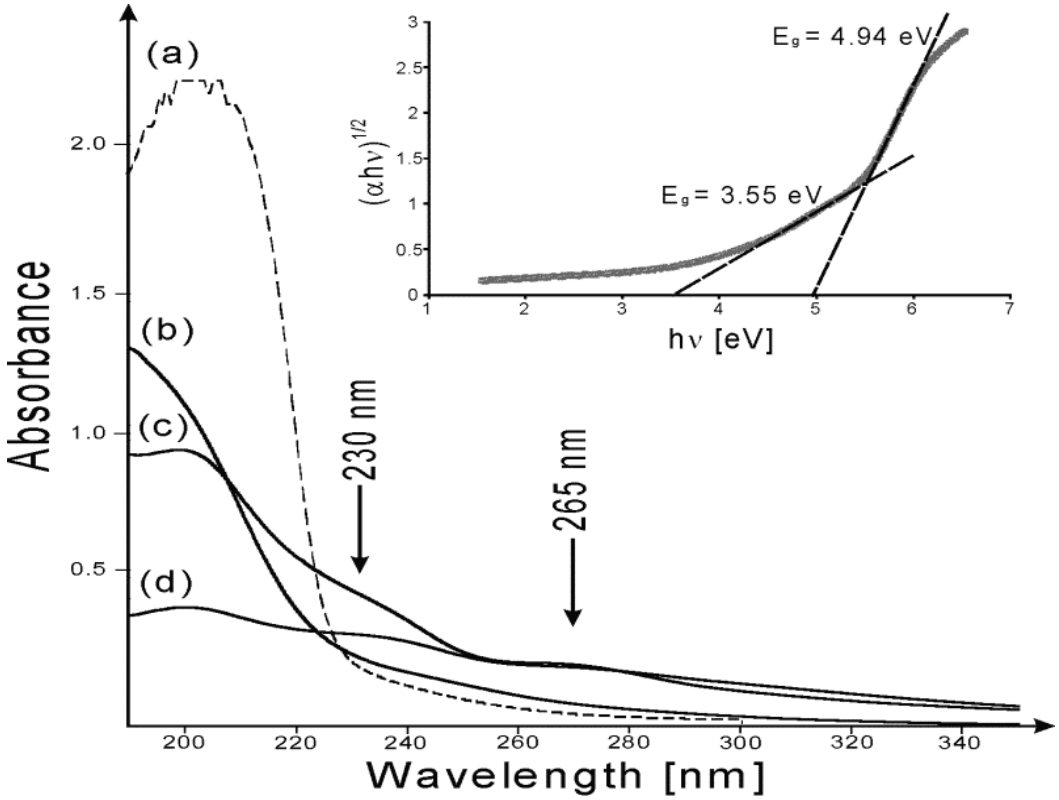
Manganese atoms diluted in silicon or germanium matrix are potential ferromagnetic semiconductors. Thin layers have been prepared by reactive excimer laser ablation of elemental manganese target under low pressure of volatile precursors (silane or germane). Ablated atoms with high energy (estimated initial temperature 1 mm above the Mn target surface is 1.9 eV) interact with gas and amorphous thin layers of Mn/Si or Mn/Ge are deposited. The prepared layers contain up to 40 % of Mn atoms. Successful crystallization was achieved by annealing of Mn/Si at as high temperatures as 1100^{o}C or rapid laser annealing using TEA CO_2 laser. Magnetic properties were studied by SQUID technique, and weak ferromagnetic properties have been revealed so far.

RIR MAPLE Procedure for Deposition of Carbon Rich Si/C/H Films

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

We applied the Resonant Infrared Matrix Assisted Pulsed Laser Evaporation (RIR MAPLE) technique to demonstrate a new approach to a controlled deposition of carbon rich amorphous Si/C/H film. In absence of radicals and accelerated species commonly generated in PECVD and sputtering setups, the RIR MAPLE method does not decompose precursor molecules. Moreover, unlike the standard MAPLE procedure, in which solvent molecules absorb laser energy from excimer or near infrared lasers, we applied the pulsed TEA CO_2 laser to excite the dendrimer precursor molecules in a frozen target. In this manner we achieved just cross-linking of the starting precursor on substrates and the deposition of carbon rich Si/C/H film. The film was analyzed by FTIR, UV/VIS, Raman and X-ray Photoelectron (XPS) spectroscopy and Atomic Force Microscopy (AFM) technique. According to analyses the film retained the precursor elemental composition free of graphitic (sp^2) clusters. In course of reaction only the peripheral allyl groups containing C=C bonds were opened to achieve cross-linking. Whereas annealing to 300 °C was necessary for the elimination of =C-H bonds in the films prepared at 200 °C, those bonds vanished completely in the films prepared at

substrate temperature 255 °C. The film possesses a smooth surface with Root Mean Square (RMS) parameter up to 10 nm within scanned distance 2.5 μm. [Ref. 7]



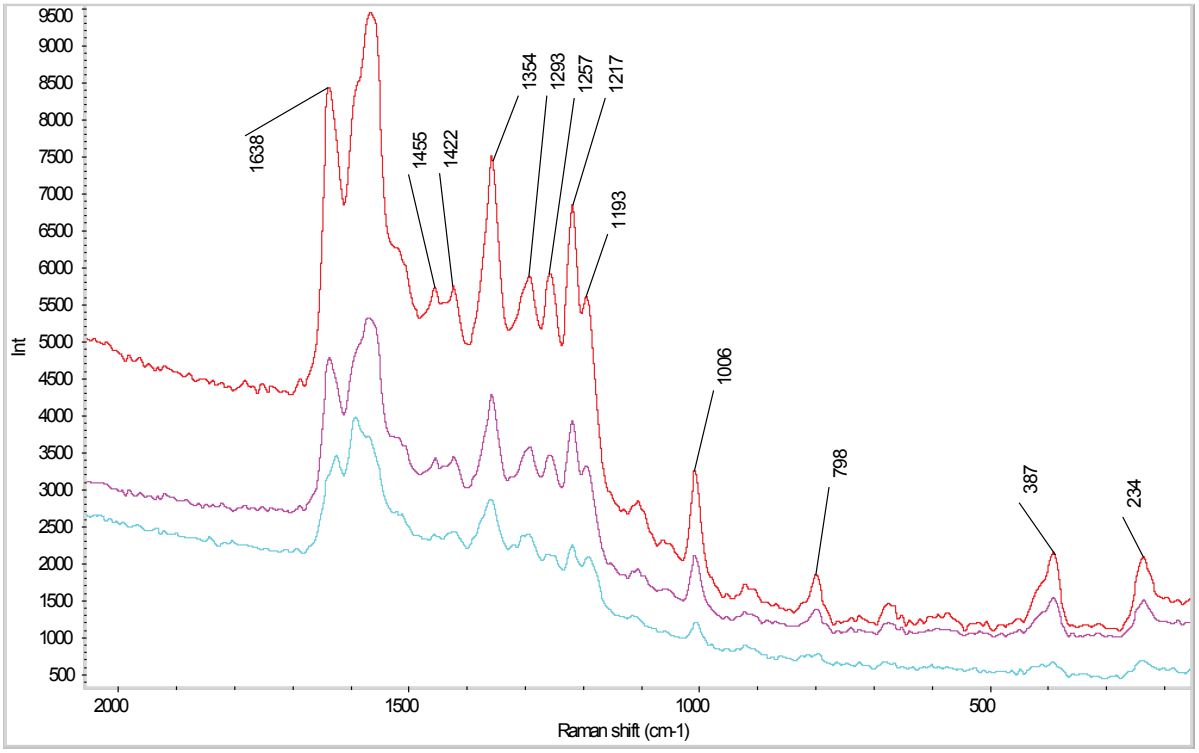
UV/VIS spectra of the (a) precursor and film prepared at 255 °C (b) before annealing and after annealing at (c) 400 and (d) 500 °C. The Tauc plot of the spectrum (b) is depicted in the inset with indicated energy gaps

Novel sensors based on laser ablated graphene

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

Graphene layer deposited by excimer laser ablation technique on a glass substrate was covered with silver nanoparticles and highly sensitive substrates for Surface-Enhanced Raman Scattering (SERS) were prepared. In vacuum, Ag nanoparticles reaching the polymer/ graphene substrates induce graphitization of the graphene sheets as revealed by Raman spectroscopy. Ablation conditions were optimized to preserve graphene layers as a substrate for Ag nanoparticles deposition in helium atmosphere. The nanocomposites were characterized by means of spectroscopy, microscopy and diffraction techniques.

The SERS substrate performance was tested using Rhodamine 6G as a probe compound. Highly enhanced signal was observed and sensoric properties of the novel substrates were demonstrated. The substrates were optimized for detection of compounds, interesting from technological and medical aspects (e.g. methylviolet B, arsenazo, beryllon).



SERS spectra of beryllon, concentration 10^{-4}, 10^{-5}, 10^{-6} mol L^{-1} (from top to bottom)

Laser-induced approach to nanoscopic titanium oxycarbides

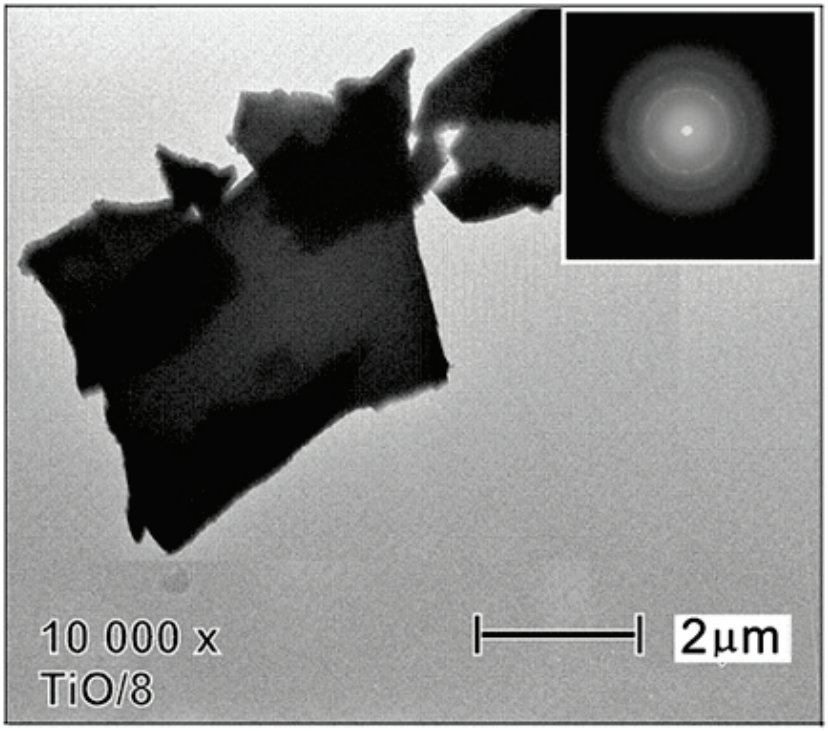
(J. Pola, pola@icpf.cas.cz and V. Jandová, jandova@icpf.cas.cz ; supported by ICPF)

IR laser-induced reactive ablation of different targets (elemental titanium, titanium monoxide and titanium ethoxide) was carried out. Ablation of hexagonal titanium in vacuum leads to amorphization of ablated Ti particles and when carried out in gaseous carbon monoxide it proceeds as reactive ablation involving particles amorphization, oxidation and carbidation.

The ablation of titanium monoxide in hydrogen was compared to the same process induced in vacuum and shown to result in deposition of hydrated surface modified nanostructured titanium suboxide films. The films exert good adhesion to metal and quartz surfaces and are hydrophobic in spite of having their surface coated with adsorbed water.

Reactive IR ablation of a frozen titanium ethoxide target (-100°C) in gaseous methane (2 to 15 Pa) proceeds as oxidation and carbidation process affording films with good adhesion and various hydrophility depending on carbon content.

The films were examined by FTIR, Raman and X-ray photoelectron spectroscopy, X-ray and electron diffraction and electron microscopy. [Refs. 2, 3, 6]



TEM image of the solid Ti/O/C film deposited in methane (8 Pa). Inset: the electron diffraction pattern, showing nanocrystalline structure of the film

Quantum size effect in semiconductor nanostructures for optoelectronics

(R. Fajgar, fajgar@icpf.cas.cz; V. Dřínek drinek@icpf.cas.cz ; cooperation with Institute of Physics of the ASCR, supported by MEYS, project No. LH12236)

Thin layers of hydrogenated silicon were prepared by excimer laser ablation of silicon target in vacuum and silane (SiH_4) atmosphere. Optical and electrical properties were studied for potential applications in light emitting devices and photovoltaic cells. Introducing of inorganic nanoparticles (PbS, Mg_2Si) into silicon layers was studied with aim to increase light scattering and absorption in solar cells. Reflection and fluorescence spectra confirm the improved light scattering of layers with embedded nanoparticles. Enhancement of optical absorption, especially at lower wavelengths was demonstrated. Combination of standard RF plasma-enhanced CVD in two electrodes configuration with reactive excimer laser ablation afforded multilayers of Mg_2Si nanoparticles encapsulated in amorphous silicon. The multilayers show an enhanced absorption in Vis-NIR spectral region. [Ref. 5]

International co-operations

Division of Nuclear Physics, Department of Physics, Lund University, Lund, Sweden
Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
Ghent University, Institute for Nuclear Sciences, Ghent, Belgium: OC/EC in urban and suburban PM10 aerosol in Prague, Hygroscopic properties of urban and suburban carbonaceous aerosols
Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan
Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, Switzerland
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behavior

Southern Illinois University Carbondale, Carbondale, IL, USA: Friction materials based on polymer matrix containing metals and their impact on environment
Technical University of Crete, Chania, Greece: Aerosols in the indoor environment
University of Helsinki, Division of Atmospheric Sciences, Helsinki, Finland
Tampere University of Technology, Tampere, Finland: Synthesis and characterization of nanosized metal/ceramic particles
University of Vienna, Faculty of Physics, Dept. of Aerosol physics and Environmental Physics, Vienna, Austria: Black and elemental carbon analysis, aerosol optical properties
Faculty of Technology and Metallurgy, University of St. Cyril & Methodius, Skopje, Republic of Macedonia: Preparation of SERS active substrates based on Ag/graphene
Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of nanosized metal chalcogenides, polycarbosilathianes and Ti based nanostructures
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
National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania: Laser-induced CVD of Fe/polymer nanocomposites
National Institute of Advanced Industrial Research and Technology, Tsukuba, Japan: Laser control of organic reactions
POLYMAT, Institute for Polymer Materials, San Sebastian, Spain: Laser ablation of graphene-based composites
AC2T, Wiener Neustadt, Austria: Tribological study of nanostructured materials (nanowires, nanoplatelets)
Institute of Automation and Control Processes of FEB RAS, Vladivostok, Russia: Deposition of magnesium silicide nanoparticles encapsulated in amorphous silicon
Institute of Atmospheric Pollution Research, Monterotondo, Italy: Gaseous pollutants

Visits abroad

D. Brus: Finnish Meteorological Institute, Helsinki, Finland (12 months)
L. Krabáč: AC2T, Austria (4 months)

Visitors

T. Hussein, University of Helsinki, Helsinki, Finland
V. Nororos, University of Helsinki, Helsinki, Finland
Gordana Siljanoska, University of St. Cyril & Methodius, Skopje, R. Macedonia
Nikolay G. Galkin, Inst. of Automation and Control Proc. of FEB RAS, Vladivostok, Russia
A. Wonaschütz, University of Wien, Faculty of Physics

Teaching

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

Publications

Original papers

[1] Beddows D.C.S., Dall'Osto M., Harrison R.M., Kulmala M., Asmi A., Wiedensohler A., Laj P., Fjaeraa A.M., Sellegri K., Birmili W., Ždímal V., Zíková N.: Variations in Tropospheric Submicron Particle Size Distributions Across the European Continent 2008–2009. *Atmos. Chem. Phys. Discuss.* 13(11), 31197–31249 (2013).

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Competence centre for biorefining research (BIORAF)

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

The project creates an interdisciplinary center with high innovation potential for sustainable utilization of renewable sources, and will bring the Czech Republic to the leading position in next-generation biorefinery within next eight years. The project links the private sector with experts from different fields of science (e.g., biosciences, phycology, analytical chemistry, enzymology, microbiology, chemical and biochemical engineering, material engineering, etc.).

Joint organizations:

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

BIORAF
Centrum kompetence pro výzkum biorafinací

Director of the Centre and project manager: Ing. Petr Kaštánek, Ph.D.

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

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

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

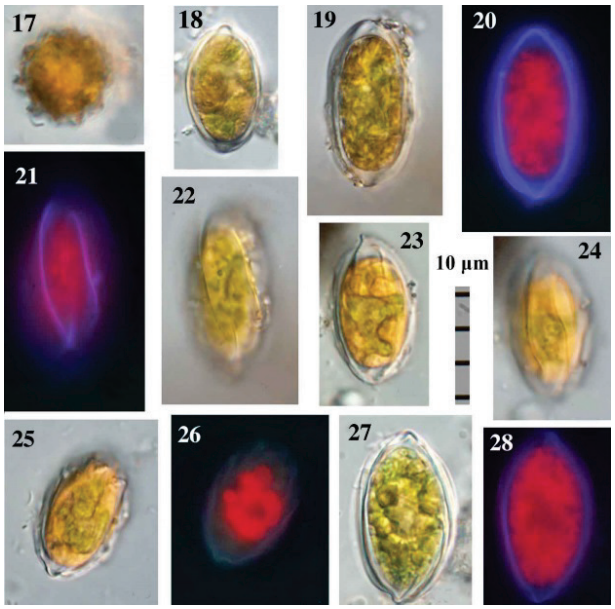
Biorefinery research centre of competence

(O. Šolcová, solcova@icpf.cas.cz)

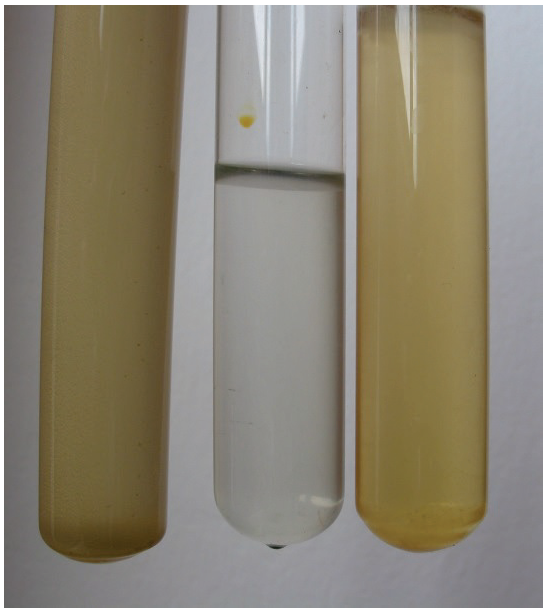
Sustainable biomass resources, which will not compete with food crops in the use of agricultural land, will be employed in the project. New environmentally friendly processes for biomass biorefining will be developed in the order to obtain products with high market value and increase the market opportunities of participating companies, which will promote job creation. New technologies will be validated in the demonstration and pilot plant units; the developed products and technological processes will be commercialized.

Within four years, new intellectual property in the field of biorefinery will be created. The transfer of know-how from research to commercial sector will help to increase innovation potential and export opportunities of the participating companies. The project will bring the lend support to the Czech agriculture and industry and attract significant long-term investment opportunities in new technologies with high socio-economic impact.

Educational programs for graduates and young scientists have been developing to create experts in emerging technologies and opportunities for their employment. Finally, the project will contribute to the independence of the Czech Republic on fossil fuels and help to reduce the emissions of greenhouse gases.



COBIEM collection



Inulin and fructose syrups

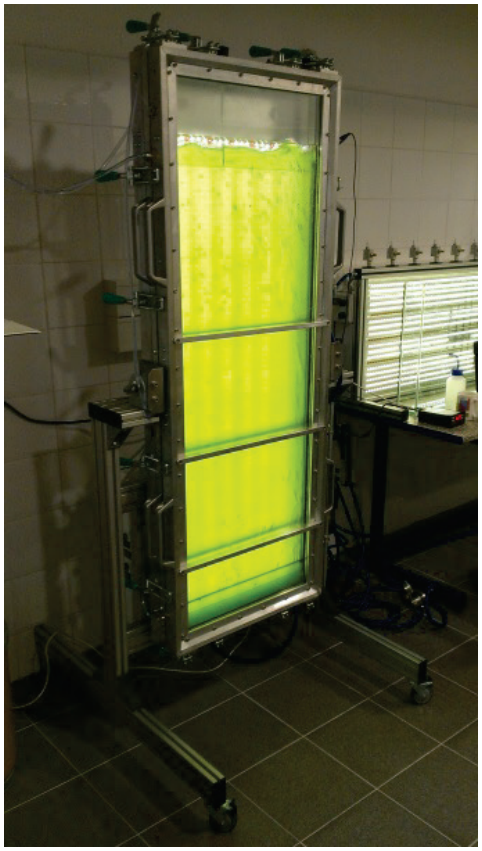


Photo-bio-reactor

Feathers as reusable materials

Method for processing algae and cyanobacteria

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

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

Sedimentation of algae

Method and device for hydrolysis of inulin solution

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

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

Method of hydrolysis of inulin from natural juice was based on membrane electrodialysis device, in which the anode compartment was fed a solution of natural juices containing inulin.

This solution was treated together with mineral salts from a previous separation of juice. In the cathode compartment provided a hydrolyzate formed in the anode compartment. [Ref. 2]

Root of topinambour and process of drying

Publications

Patents

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15TH E. HÁLA LECTURE (2013)

CHRISTOPHER HARDACRE (School of Chemistry and Chemical Engineering, Queen's University, Belfast, Northern Ireland, UK), on 4 November 2013:
"Ionic liquids - from Structure to Application"

ACRONYMS USED THROUGHOUT THE REPORT

ASCR	Academy of Sciences of the Czech Republic
BAS	Bulgarian Academy of Sciences
CFD	Computational Fluid Dynamics
CFL	Compact Fluorescent Lamp
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
GA ASCR	Grant Agency of Academy of Sciences of the Czech Republic
HDS	Hydrodesulfurization
IBOT	Institute of Botany of ASCR, v. v. i., Průhonice
ICPF	Institute of Chemical Process Fundamentals of the ASCR, v. v. i., Prague
ICT	Institute of Chemical Technology, Prague
IIC	Institute of Inorganic Chemistry of the ASCR, v. v. i., Prague
IL	Ionic Liquid
IMC	Institute of Macromolecular Chemistry of the ASCR, v. v. i., Prague
IR	Infrared
JH IPC	J. Heyrovský Institute of Physical Chemistry of the ASCR, v. v. i., Prague
KIT	Karlsruhe Institute of Technology
LC	Liquid Chromatography
LDH	Layered Double Hydroxide
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
UJEP	Jan Evangelista Purkyně University in Ústí nad Labem, Czech Republic
UV	Ultraviolet
VOCs	Volatile Organic Compounds
VÚAnCh	Research Institute of Inorganic Chemistry, Inc., Ústí nad Labem
XRD	X-ray Diffraction

Annual Report 2013

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