INTITUTE 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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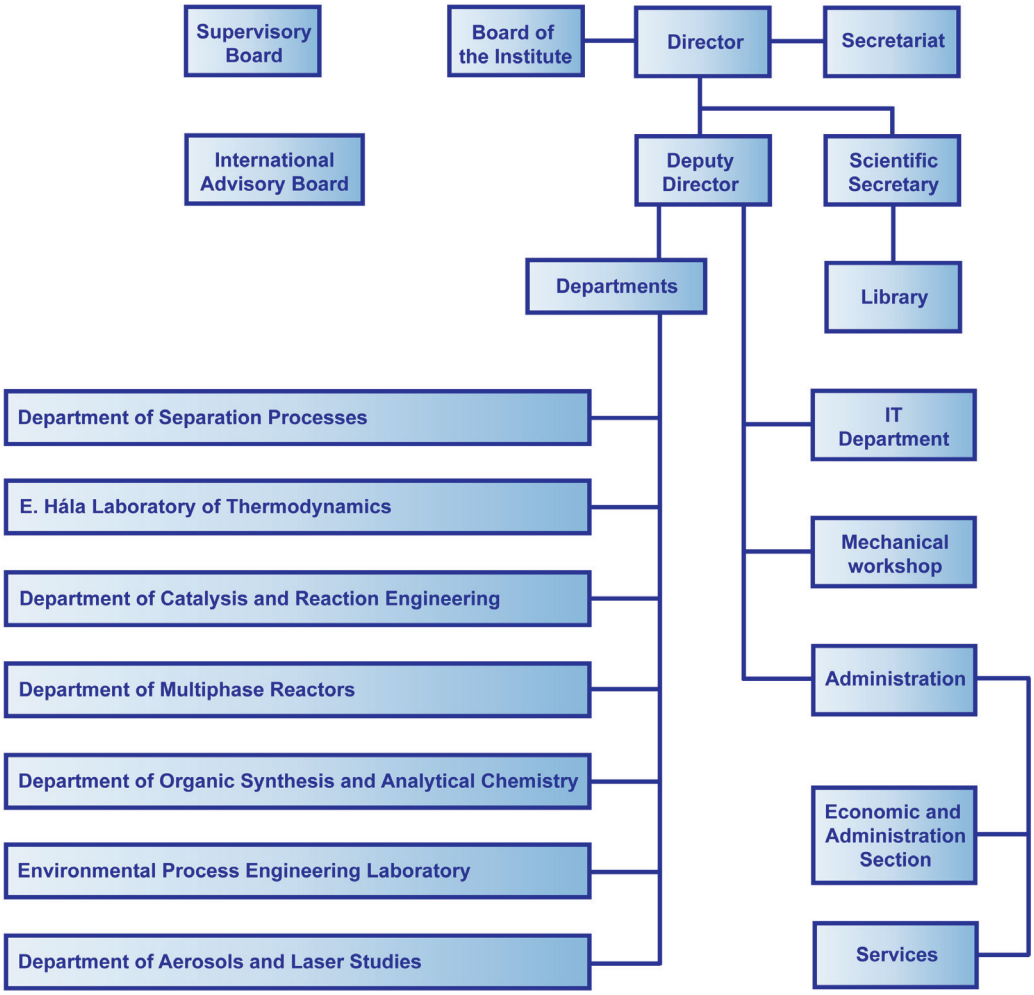

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STAFF

(December 31, 2012)

Category	Number of Employees
Research	144
Technical	10
Administrative	14
Services	12

BUDGET 2012

(19.05 CZK ≈ 1 US$, 25.14 CZK ≈ 1 €)

Resources	Million CZK
Institutional support based on Institutional Research Plan	81
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	54
Foreign R&D Funds and European Programmes	7
Contracts with industry	3
Other resources	24
Total Resources	**169**

Expenses	Million CZK
Personal expenses including mandatory insurance	90
Purchase of material	13
Purchase of services	10
Repairs and maintenance	16
Depreciation of fixed assets	19
Travel expenses	4
Energy, water, and fuels	6
Total other expenses	11
Total other expenses	**169**

Department of Separation Processes

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LAB TECHNICIANS
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Fields of research

- Hydrodynamics of two phase flow in micro 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
- Chemical and enzymatic reactions in supercritical CO_2
- Mass transport through ionic liquid membranes
- Membrane separation of methane and CO_2
- Separation of racemic mixtures
- Separation of gasoline vapors from air by supported ionic liquids membranes
- Condensation in porous membranes during vapor permeation

Applied research

- Hydrodynamic characterization of micromixers
- Heat and mass transfer of liquid flow in microreactors
- 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

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. The installation of microsulphonator into Procter&Gamble pilot plant is foreseen for early 2013. ICPF team also defined an advanced method for the SO_2 analysis suitable for the pilot plant installation. We also participated in the design of pilot plant size microreactor for sulfur dioxide catalytic heterogeneous oxidation.

Gas-liquid electrochemical microreactors - role of hydrodynamics

(J. Křišťál, kristal@icpf.cas.cz; bilateral project ASCR-CNRS, project No. 22540)

The proposed project deals with the study of hydrodynamics of the gas-liquid flow generated by an electrochemical reaction in a low aspect ratio microreactor. Objective is to better understand and characterize the effect of gas flow and bubbles on the performance of liquid electrochemical reactions being performed in the electrochemical microreactor. [Ref. 14]

Schematic diagram of the T-junction microchannel (left) and the topology of the curved (center) and right-angled (right) meandering microchannels

Refining of biologically active therapeutic substances from coniferous wood

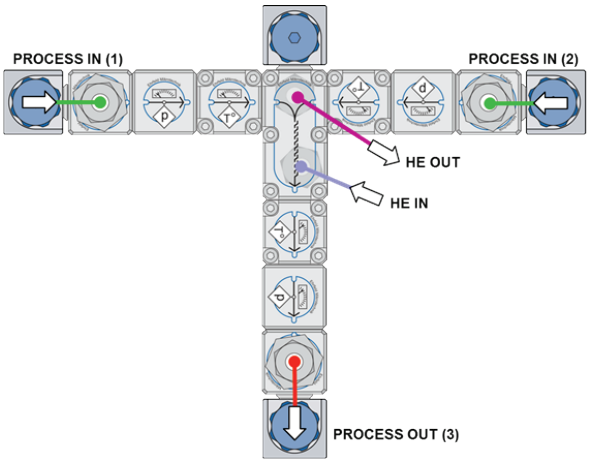
(A. Heyberger, heyberger@icpf.cas.cz; contract with Favea Europe Ltd.)

The object of this contract was to perform laboratory and pilot plant tests for refining of liquid coniferous extracts using countercurrent vibrating plate extractor (VPE). The experimental results were used as a basis for the design of the operating extractor to replace the existing batch production.

Research and developments of various microapparatus characteristics

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

The contract deals with experimental measurement of various microapparatuses (preferably mixers) and determination of their hydrodynamic characteristics with respect to various physical-chemical properties selected liquids. The collected data and developed methodology of micromixer selection will form databasis for design and development of new chemical processes. Results published in three confidential Procter&Gamble research reports.



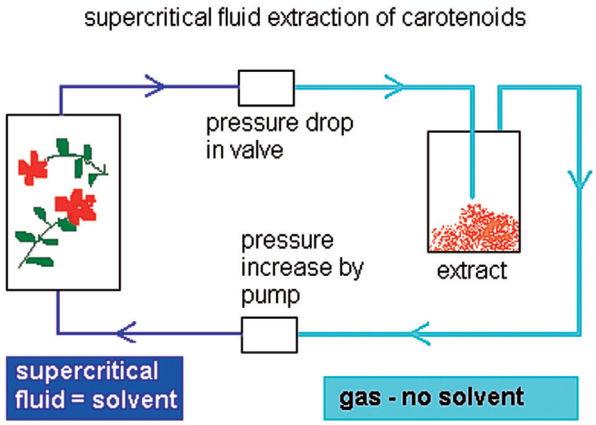
Visualization of the experimental set-up for testing of micro mixers

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. 2, 9-12]



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)

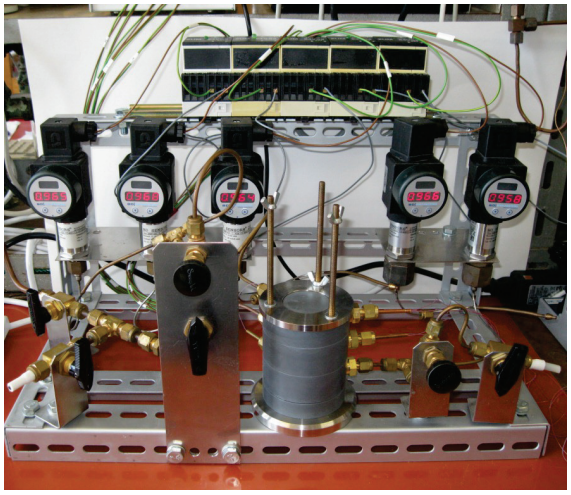
The location of the phase change inside membranes and swelling of the membrane material during toluene transport in a polyethylene membrane were investigated. The special

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. [Ref. 15]

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)

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

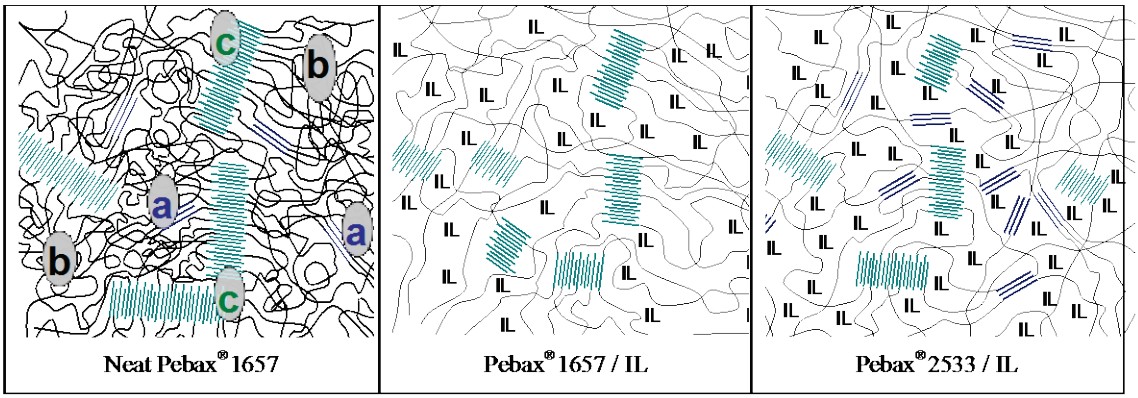


Apparatus for vapor permeation transport connected with condensation

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. Optimization of polymeric membrane for specific separation task is time consuming and financial demanding. Ionic liquids have a great potential for membrane processes especially if only a small amount of ionic liquid is necessary e.g. supported ionic liquid membranes (SILMs). Characteristic property of ionic liquid is their very low vapor pressure, which makes them attractive for gas and vapor permeation. [Refs. 1, 4, 5, 6, 8]



Schematic representation of the microstructure of pure Pebax® (left), Pebax®1657/IL gel (middle), and Pebax®2533/IL gel (right). Domain identification: a = crystalline PE blocks; b = amorphous soft PE blocks and amorphous hard PA blocks, c = crystalline hard PA blocks, IL = dissolved [BMIM][OTf]

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)

Drug stereochemistry has become an issue for the pharmaceutical industry and the regulatory authorities, because each of the enantiomers frequently shows different impacts to living organisms. 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. To greatly reduce the amount of experimental work, particle-based modeling will be employed. After gathering all transport characteristics, it will be possible to model the separation process and to estimate permeability and selectivity of the separation.

International co-operations

CNRS Toulouse, France: Two phase flow hydrodynamics in microchannels

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

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: Mass transport through porous membranes
Procter&Gamble, Belgium: Research and developments of microapparatus characteristics
Procter&Gamble: Hydrodynamics of micro reactor for sulfonation
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, CNRS, Toulouse, France (1 week)
P. Uchytil, National Chung Hsing University, Taichung, Taiwan (3 weeks)
A. Heyberger, University of KwaZulu-Natal, Durban, Republic of South Africa (3 weeks)

Visitors

J. Aubin, CNRS Toulouse, France
A. Bucić-Kojić, Faculty of Food Technology, Osijek University, Croatia
M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
J. Heck, C. Raffa, Ehrfeld Mikrotechnik BTS, Germany
A. Palavra, Technical University of Lisbon, Portugal
A. Martin, ENSIASET, Toulouse, France
A. Simmoncelli, Procter&Gamble, Belgium
R.P. Stateva, Inst. Chem. Eng. BAN, Sofia, Bulgaria

Teaching

P. Izák: ICT, Faculty of Chemical Engineering, postgraduate course “Physical chemistry for technological practice”
J. Hanika: ICT, Faculty of Chemical Technology, postgradual course “Multiphase reactors”
J. Hanika: ICT, Faculty of Chemical Technology, course “Pharmaceutical engineering”
H. Sovová: ICT, Faculty of Chemical Engineering, postgraduate course “Properties and application of supercritical fluids”

Publications

Original papers

[1] Bernardo P., Jansen J.C., Bazzarelli F., Fuoco A., Friess K., Izák P., Jarmarová V., Kačírková M., Clarizia G.: Gas Transport Properties of PEBAX®/Room Temperature Ionic Liquid Gel Membranes. *Sep. Purif. Technol.* 97(SI), 73-82 (2012).

[2] Coelho J.P., Cristino A.F., Mantos P.G., Rauter A.P., Nobre B.P., Mendes R.L., Barroso J.G., Mainar A., Urieta J.S., Fareleira J.M.N.A., Sovová H., Palavra A.F.: Extraction of Volatile Oil from Aromatic Plants with Supercritical Carbon Dioxide: Experiments and Modeling. *Molecules* 17(9), 10550-10573 (2012).

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[5] Izák P., Kárászová M., Vejražka J., Friess K., Randová A., Jansen J.C.: The Effective Upgrading of Raw Biogas to Methane by Selective Membranes. *Procedia Eng.* 44, 429-431 (2012).

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[7] Křišťál J., Kodym R., Bouzek K., Jiřičný V., Hanika J.: Electrochemical Microreactor Design for Alkoxylation Reactions – Experiments and Simulations. *Ind. Eng. Chem. Res.* 51(4), 1515-1524 (2012).

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[13] Vajglová Z., Veselý M., Křišťál J., Vychodilová H., Tříska J., Jiřičný V.: Photochemical Degradation of Polybrominated Diphenyl Ethers in Micro Photo-Reactor. *Procedia Eng.* 42(SI), 1378-1382 (2012).

[14] Záloha P., Křišťál J., Jiřičný V., Völkel N., Xuereb C., Aubin J.: Characterisation of Liquid Slugs in Gas-Liquid Taylor Flow in Microchannels. *Chem. Eng. Sci.* 68(1), 640-649 (2012).

[15] C.-Y. Liang, P. Uchytil, R. Petrychkovych, Y.-C. Lai, K. Friess, M. Sipek, M. M. Reddy, S.-Y. Suen, Preparation of PES (polyethersulfone)/MMT (Na-montmorillonite) and PES/TiO2 mixed matrix membranes for CO2/CH4 separation, Sep. Purif. Technol. 92, 57-63 (2012).

Chapters in books

[16] Hanika J.: Chemie na konci světa. (Czech) Chemistry in Ending World. In: Tři svíce za budoucnost. (Cílek, V., Ed.), pp. 44-54, Novela bohemica, Praha 2012.

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Patents

[19] Izák P., Kárászová M., Vejražka J.: Způsob separace plynné směsi a zařízení k provádění tohoto způsobu. (Czech) A Process for the Separation of a Gaseous Mixture and an Apparatus for Carrying Out the Same. Pat. No. CZ303107/PV 2010-438. Applied: 11.06.20, patented: 12.04.04.

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E. Hála Laboratory of Thermodynamics

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LENKA MORÁVKOVÁ

PHD STUDENTS
ADÉLA ANDRESOVÁ, KAROLINA MACHANOVÁ, STANISLAV PAŘEZ

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

Applied research

- Technology for the preparation of molecularly imprinted polymeric materials

Research projects

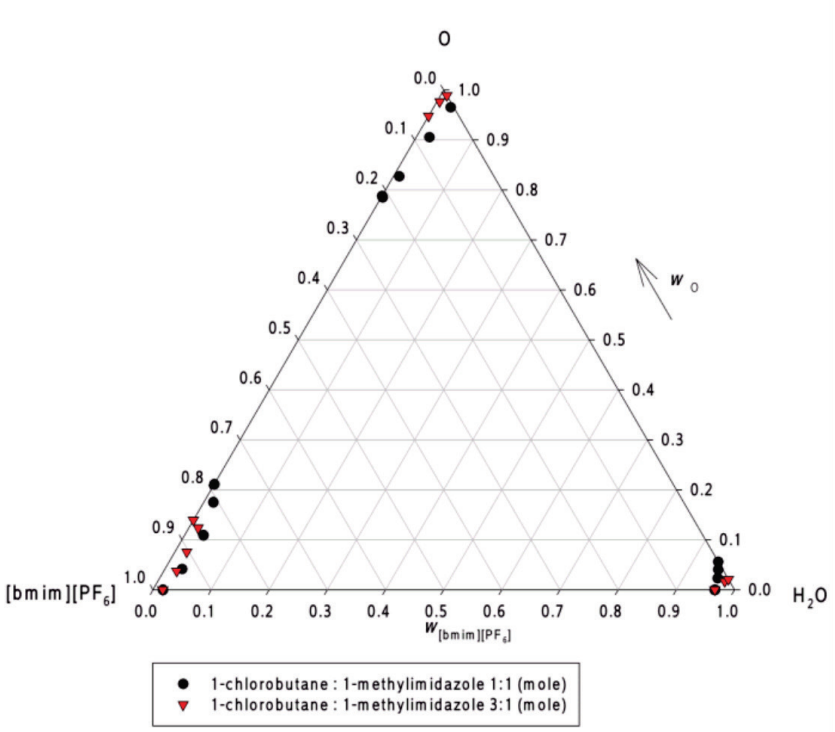
Properties of ionic liquids - experiment and modelling

(M. Bendová, Z. Wagner, bendova@icpf.cas.cz, wagner@icpf.cas.cz; joint project with Queen's University of Belfast, UK and Université Blaise Pascal, France; supported by MEYS, project No. LG12032 and by ICPF)

Ionic liquids (ILs) have been extensively studied for more than two decades now by a number of research teams worldwide. This ever growing class of compounds still remains largely uncharacterized in terms of their thermodynamic properties. To be able to use ionic liquids efficiently in any application, knowledge of their properties as pure compounds and in mixtures with molecular compounds is necessary. A wide range of thermodynamic and physical properties, such as density, viscosity, excess properties and phase behavior is studied not only to facilitate scale-up from a lab bench to a pilot plant, but also to understand the underlying structural effects that influence on the studied macroscopic properties.

Experimentally, thermal properties (heat capacity and phase transitions) in pure ILs using differential scanning calorimetry (DSC) are studied in our group. In mixtures of ILs with molecular solvents, liquid phase behavior is investigated using the following methods:

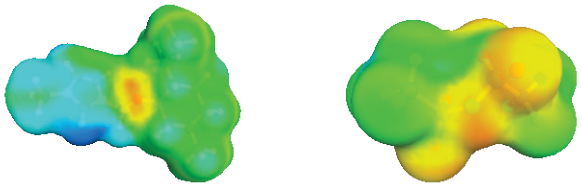
- cloud-point (nephelometric, synthetic) method [8]
- direct-analytical method [1]
- volumetric method [8]



Miscibility gaps in pseudoternary systems 1-butyl-3-methylimidazolium hexafluorophosphate + H_2O + (1-chlorobutane/1-methylimidazole) determined by the cloud-point method

To obtain useful data for the assessment of impact of the studied ionic liquids on environment, the above-mentioned methods are used to measure their mutual solubility with water and 1-octanol and the partitioning coefficient octanol/water K_{OW}. These experiments enable us to assess their hydrophobicity/lipophilicity and hence their tendency to bioaccumulation.

At the same time, experimental work combined with appropriate modelling leads us to a deeper understanding of the influence of the structure of the ionic liquid on its properties. Experiments are complemented with modelling using the COSMO-RS methodology that uses quantum chemistry combined with continuum solvation models for a priori predictions of chemical potentials. Description of experimental data using SAFT-type equations of state provides us with an insight into the molecular structure of the pure ionic liquids and their mixtures. [Refs. 1, 3, 8]



(a) (b)

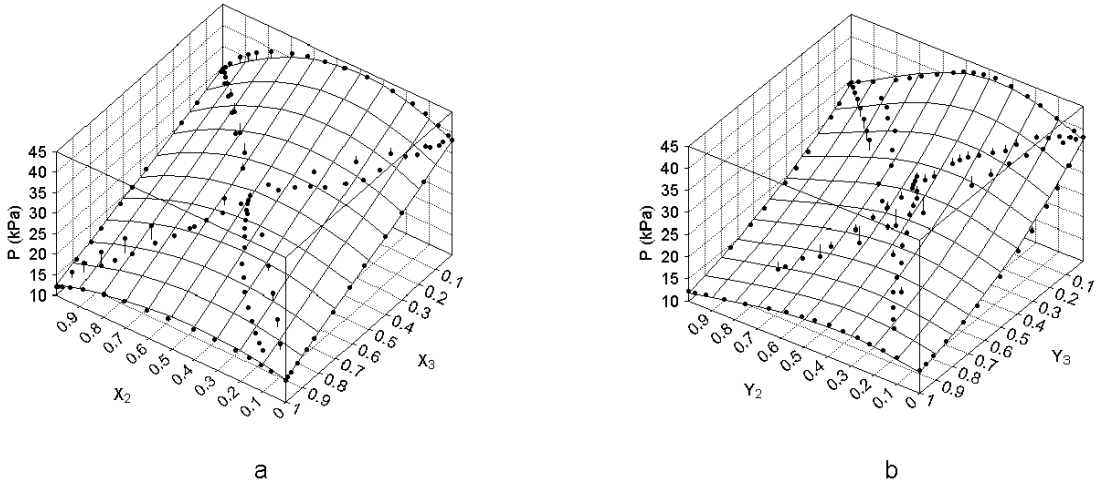
Screening charge density of 1-[(1*R*, 2*S*, 5R)-(–)-menthoxymetyl]-3-methylimidazole cation (a) and bis(trifluoromethanesulfonyl)imide anion (b) using COSMO methodology

Vapor-liquid equilibria and thermodynamic properties - experiment and data processing

(I. Wichterle, Z. Sedláková, wichterle@icpf.cas.cz, sedlakova@icpf.cas.cz; supported by ICPF)

a) Systems containing low molecular mass components

Isothermal vapor-liquid equilibrium (VLE) data were measured in binary and ternary systems containing alcohol, hydrocarbon and ketone, namely 2-propanol, isooctane, and 2,4-dimethyl-3-pentanone. The binary VLE data were correlated using the Wilson and nonrandom two-liquid (NRTL) equations by means of a new algorithm and resulting parameters were then used for the calculation of phase behavior in the ternary system and for subsequent comparison with experimental data. Phase and chemical equilibria were isothermally determined in system with chemical reaction (transesterification), namely in the quaternary ethyl ethanoate + ethanol + propyl ethanoate + propanol system and in all six binary subsystems. Good prediction was achieved with use of evaluated NRTL binary parameters; deviations are shown in Figure. [Refs. 11, 12]



Modified composition variables versus pressure for the ethyl ethanoate (1) + ethanol (2) + propyl ethanoate (3) + propanol (4) system at 348.15 K; (a) liquid phase; (b) vapor phase

b) Systems containing polymers

Vapor-liquid equilibria have been determined in the systems composed of polyacrylic acid with water, and poly(methyl methacrylate) with acetone by ebulliometric (total pressure measurement) method. Ebulliometer has been redesigned (see Figure) and experimental procedure has been upgraded. Experiments have been carried out isothermally and the measured data were correlated by the UNIQUAC equation, and compared with available data. Results were presented at two international conferences.

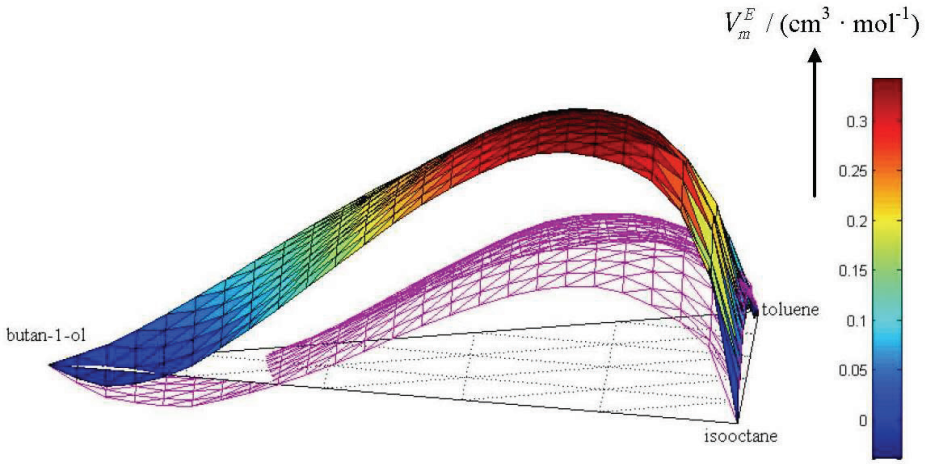
New design of microebulliometer

c) Prediction of properties of petroleum fluids

A simplified method for characterizing petroleum fluids (crude oil and gas condensate) and for predicting phase equilibria was developed. Vapor-liquid equilibria in such highly complex natural mixtures were calculated by the pseudo-component method, which assumes that each fraction is a mixture of predefined pure components. The required input data include complete TBP (true boiling point) analysis, PNA (paraffin-naphthene-aromatic hydrocarbon) analysis, and density data, preferably for each sub-fraction. Known thermodynamic procedures are used to estimate the critical data, acentric factor, and molecular weight for the model compounds. [Refs. 2, 13]

d) Molar excess volumes

Experimental determination of molar excess volumes in the benzene + *tert*-amyl methyl ether + isooctane and the isooctane + toluene + butan-1-ol systems have been carried out. Data were successfully correlated by means of the ERAS model and the Redlich-Kister equation.



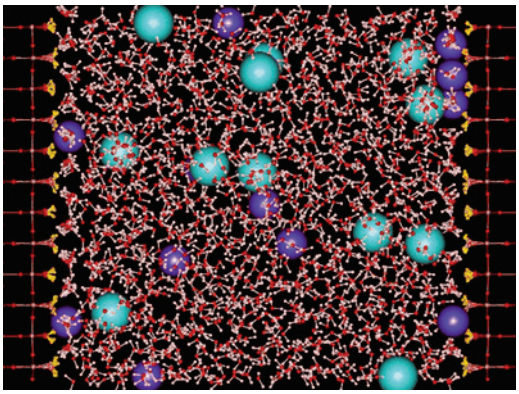
Excess molar volume for the ternary isooctane + toluene + butan-1-ol system at temperature 298.15 K (violet net) and 328.15 K (in colors)

Molecular based studies of fluid systems

(S. Pařez, M. Předota, A. Malijevský, I. Nezbeda, M. Lísal, parez@icpf.cas.cz, predota@icpf.cas.cz, malijevsky@icpf.cas.cz, nezbeda@icpf.cas.cz, lisal@icpf.cas.cz; joint with University of South Bohemia, Ceske Budejovice, with ICT and Imperial College London, UK, and with UJEP; supported by MEYS, KONTAKT II, project No. LH12020, by GA ASCR, projects No. IAA400720802 and IAA200760905, and by GACR, project No. P106/10/1194)

(a) Solid-liquid interfaces

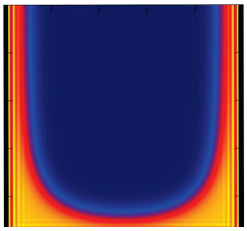
Shear viscosity and relative permittivity of aqueous mixtures were studied in the interfacial region at a planar surface. Profiles of both properties show significant deviations from their bulk values when approaching the surface. Our simulation results provide pieces of information inaccessible by experiment that promote our understanding of peculiar properties of solid-liquid interfaces. [Ref. 10]



Water/ions-TiO_2 interface

(b) Confined fluids

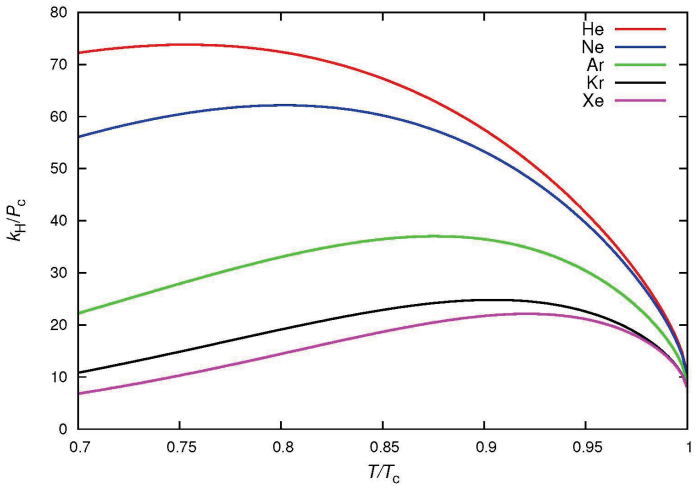
The structural and interfacial properties of a nanoscopic liquid drops and bubbles were examined by means of mechanical, thermodynamical, and statistical mechanical approaches. A novel method based on a microscopic density functional theory for calculation of surface tension and Tolman's length of highly curved interfaces was proposed. Further, phase transitions in a microscopic capillary capped at one end were studied by means of fundamental measure density functional theory. [Refs. 16, 18]



An example of microscopic capillary capped at one end

(c) Model fluids

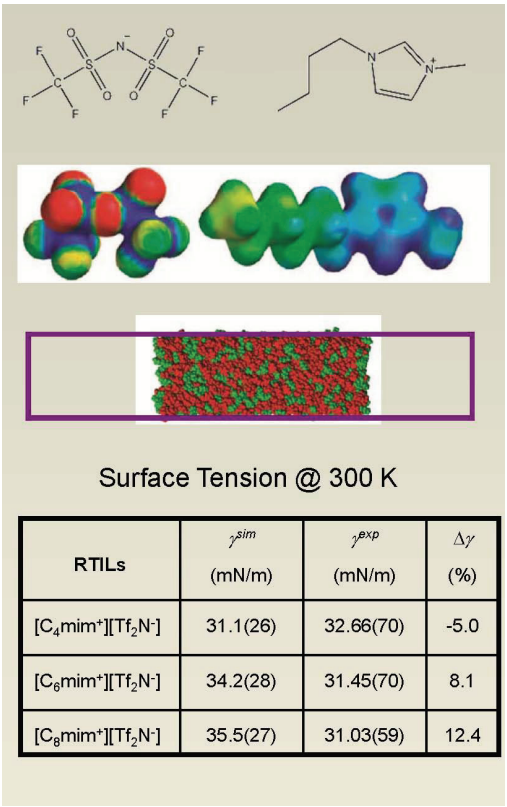
A theoretical, molecular-based model for hydration of simple nonpolar solutes has been developed. The model qualitatively reproduces basic features of hydrophobic hydration and temperature dependence of Henry's law constants of noble gases. [Refs. 4, 15]



The reduced Henry's law constant of noble gases predicted by a theoretical model based on simple interaction potentials

(d) Ionic liquid interfaces

Molecular dynamics simulations were employed to provide insight into the air-liquid interface for three ILs with a common anion: bis(trifluoromethylsulfonyl) imide, and imidazolium-based cat ions that differ in the alkyl tail length. The air-liquid interface was analyzed using the intrinsic method and of structural and dynamic properties of the interfacial, sub-interfacial and central layers were determined. [Refs. 5, 9]



Surface Tension @ 300 K

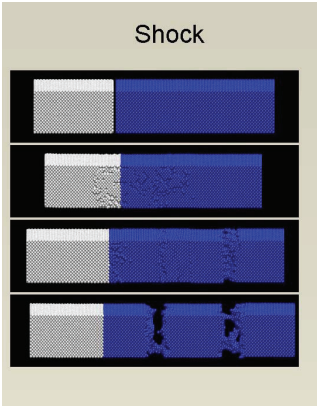
RTILs	γ^{sim} (mN/m)	γ^{exp} (mN/m)	$\Delta\gamma$ (%)
$[C_4mim^+][Tf_2N^-]$	31.1(26)	32.66(70)	-5.0
$[C_6mim^+][Tf_2N^-]$	34.2(28)	31.45(70)	8.1
$[C_8mim^+][Tf_2N^-]$	35.5(27)	31.03(59)	12.4

Molecular dynamics simulations of ILs

Mesoscale simulation studies of polymeric and energetic materials

(M. Lísal, lisal@icpf.cas.cz; joint with US Army Research Laboratory, Aberdeen, USA and Penn State University, State College, USA; supported by MEYS, KONTAKT II, project No. LH12020 and US/CZ bilateral project W911NF-10-2-0039)

Dissipative particle dynamics simulations were used to study structural and dynamic properties of entangled polymer melts. Mesoscale modelling capability is being develop for studying the dynamic response of reactive materials. [Ref. 14]



Response of Al/Ni energetic material to shock

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

Visits abroad

M. Lísal: University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)

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)

S. Pařez: University of Paderborn, Institute of Thermodynamics and Energy Technology, Paderborn, Germany (3 months)

L. Vlček: Vanderbildt University, Nashville, TN, USA (12 months)

Visitors

A. Archer, University of Loughborough, Loughborough, UK
D. Gheorghe Chiscan, Institute of Physical Chemistry I. Murgulescu, Romanian Academy of Sciences, Bucuresti, Romania
D. Dragoescu, Institute of Physical Chemistry I. Murgulescu, Romanian Academy of Sciences, Bucuresti, Romania

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" and "Introduction to a modern theory of phase transitions"
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] Bendová M., Sedláková Z., Andresová A., Wagner Z.: Using Partial Least-Squares Regression in Multivariate UV Spectroscopic Analysis of Mixtures of Imidazolium-Based Ionic Liquids and 1-Methylimidazole for Measurements of Liquid-Liquid Equilibria. *J. Solution. Chem.* 41, 2164–2172 (2012).

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[4] Krejčí J., Nezbeda I.: The Critical Temperature and Properties of Real Gas from Low Order Perturbed Virial Expansions. *Fluid Phase Equilib.* 314, 156–160 (2012).

[5] Lísal M., Posel Z., Izák P.: Air-Liquid Interface of Imidazolium-Based [Tf_2N^-] Ionic Liquids: Insight from Molecular Dynamics Simulations. *Phys. Chem. Chem. Phys.* 14, 5164–5177 (2012).

[6] Machanová K., Boisset A., Sedláková Z., Andresová A., Jacquemin J., Bendová M.: Termodynamické vlastnosti směsí iontových kapalin a molekulárních rozpouštědel pro využití v dvoufázové katalýze. (Czech) Thermodynamic Properties of Mixtures of Ionic Liquids and Molecular Solvents for Biphasic Catalysis. *Inovační podnikání a transfer technologií*, příloha 20, V–VII (2012).

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[9] Moučka F., Lísal M., Smith W.R.: Molecular Simulation of Aqueous Electrolyte Solubility. 3. Alkali-halide Salts and Their Mixtures in Water and in Hydrochloric Acid. *J. Phys. Chem. B* 116, 5468–5478 (2012).
[10] Pařez S., Předota M.: Determination of the Distance-Dependent Viscosity of Mixtures in Parallel Slabs Using Non-Equilibrium Molecular Dynamics. *Phys. Chem. Chem. Phys.* 14, 3640–3650 (2012).
[11] Pavlíček J., Bogdanić G., Wichterle I.: Vapour–Liquid and Chemical Equilibria in the Ethyl Ethanoate + Ethanol + Propyl Ethanoate + Propanol System Accompanied with Transesterification Reaction. *Fluid Phase Equilib.* 328, 61–68 (2012).
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[14] Sirk T.W., Slizoberg Y.R., Brennan J.K., Lísal M., Andzelm J.W.: An Enhanced Entangled Polymer Model for Dissipative Particle Dynamics. *J. Chem. Phys.* 136, 134903 (2012).
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[16] Malijevský A.: Does Adsorption in a Single Nanogroove Exhibit Hysteresis*? J. Chem. Phys.* 137, 214704 (2012).

Review papers

[17] Sedláková Z., Wagner Z.: High-Pressure Phase Equilibria in Systems Containing CO_2 and Ionic Liquid of the $[C_n mim][Tf_2N]$ Type. *Chem. Biochem. Eng. Q.* 26, 55–60 (2012).
[18] Malijevský A., Jackson G.: A Perspective on the Interfacial Properties of Nanoscopic Liquid Drops. *J. Phys.: Condens. Matter* 24, 464121 (2012).

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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. 39]

Detail of reactor filled up by sand with the prepared slot for sorbents

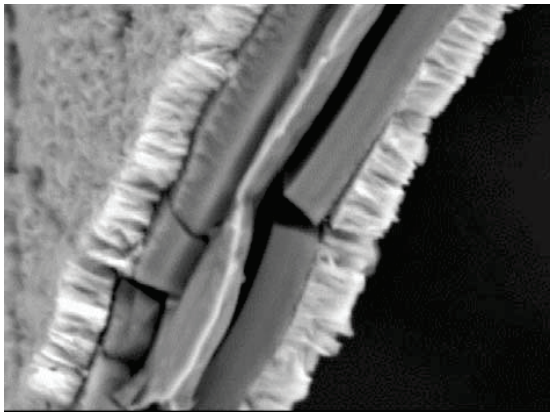
Structured catalysts with low concentration of active components for total oxidation of VOC

(K. Jirátová, jiratova@icpf.cas.cz; joint project with ICT and IIC; supported by GACR, project No. 106/10/1762)

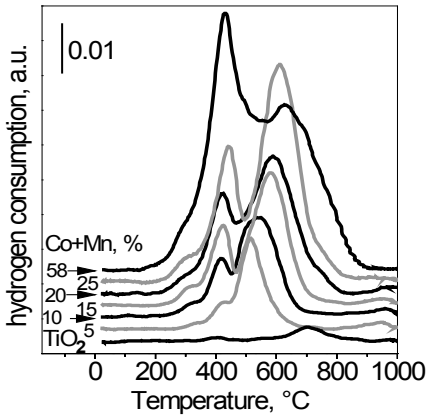
Oxide catalysts containing various combinations of Cu, Co, Ni, Mn, and Al, grained or supported on oxidized aluminum foil Al_2O_3/Al, were studied in terms of their chemical and physical properties, and activity in total ethanol oxidation. Ternary co-precipitated catalysts in the form of grains obtained from layered double hydroxide-like precursors were highly active, especially those containing manganese. Deposition of the selected precursors on an anodized aluminum foil-support afforded less active catalysts, mainly because the required metal molar ratios were not achieved, and insufficient metal amounts were deposited. However, by controlling the preparation conditions (pH), higher loading of active components and higher catalytic activity were obtained.

Catalytic activity of the Co-Mn-Al mixed oxide catalyst (Co:Mn:Al molar ratio of 4:1:1) supported over titania was examined in total oxidation of ethanol. The catalysts activity gradually increased with increasing active phase content. Low concentration of Co-Mn-Al oxides in the catalyst negatively affected formation of reaction byproducts: carbon monoxide production steeply increased when Co+Mn metals concentration were lower than 5 wt. %. On the other hand, formation of the second main reaction intermediate, acetaldehyde was limited, when acidity of the catalyst was not high, i.e. concentration of Co+Mn metals over titania was low.

Physical-chemical properties of the catalysts containing precious metals, like reducibility, acidity, basicity, and of metal specific surface area were also studied. [Refs. 20, 21, 26, 30, 31]



Scanning electron microscope image of an LDH-type Co-Mn-Al precursor grown on an Al_2O_3/Al support



Temperature programmed reduction curves of the supported Co-Mn-Al catalysts having various amounts of active components (Co+Mn) on titania

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.

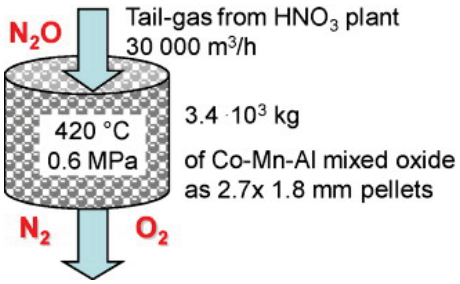
Therefore, the main objective of the project is to develop a family of advanced nanofiltration (NF) and UF ceramic composite membranes containing functionalized mesoporous silica layers which will be capable of selective binding of heavy metals (Hg, Cd, Cr) and uranium from surface and waste waters and thus preventing or minimizing the environmental exposure to hazardous substances. [Refs. 37, 38]

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

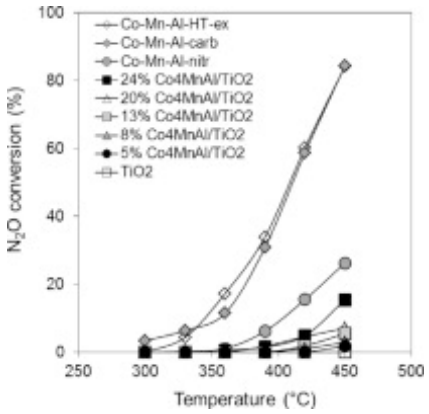
(K. Jirátová, jiratova@icpf.cas.cz; joint project with TU of Ostrava, and ICT; supported by TACR, project No. TA01020336)

Pilot reactor for low temperature N_2O decomposition in off-gases from HNO_3 production was designed. Pseudo-homogeneous one-dimensional model of an ideal plug flow reactor was used for modeling of N_2O decomposition in a laboratory fixed bed reactor filled with grains or pellets of a Co–Mn–Al mixed oxide catalyst. Increase in inlet pressure up to 0.6 MPa did not influence the effective diffusion coefficient, but improved the achieved N_2O conversion. Based on the laboratory data of N_2O decomposition over Co–Mn–Al mixed oxide pellets, catalyst bed of 3400 kg was estimated for target 90% N_2O conversion (30 000 $m^3\ h^{-1}$ of exhaust gases from HNO_3 plant containing 0.1 molar% N_2O, 0.01 molar% NO, 0.01 molar% NO_2, 3 molar% H_2O, 5 molar% O_2) at 420°C and 600 kPa inlet pressure.

A series of Co–Mn–Al/TiO_2 catalysts with different Co+Mn loading (5–24 wt. %) was prepared by impregnation of TiO_2 support and compared with bulk Co–Mn–Al mixed oxides. TiO_2 acted only as a catalytic support and did not contribute to the catalytic activity. The N_2O conversion over TiO_2-supported Co–Mn–Al catalysts was increasing with Co + Mn loading, and was proportional to the amount of easily reducible components. Comparing the catalysts with identical amount of active components, the highest catalytic activity was achieved on the calcined precursors having carbonates in their molecules (layered double hydroxides Co–Mn–Al-HT-ex and Co–Mn–Al-carb), the lowest one on the calcined Co–Mn–Al nitrates due to the lower surface area, less advantageous porous structure and worse reducibility. [Refs. 12, 27]



Scheme of the reactor arrangement for N_2O decomposition



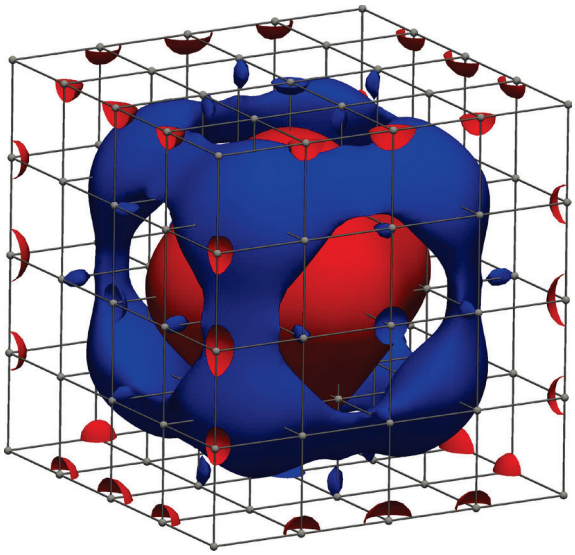
Temperature dependence of N_2O conversion over Co–Mn–Al mixed oxide supported on TiO_2. Conditions: 0.1 mol % N_2O balanced in He, 0.1 MPa, GHSV = 60 l g^{-1} h^{-1}

Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, rponec@icpf.cas.cz; joint project with University of Pécs, Hungary, University of Girona, Spain; supported by GACR, project No. 203/09/0118)

The project is a part of longer-term efforts at the systematic exploitation of the pair density as new source of the information about the molecular structure and nature of chemical bond. This density represents the basic theoretical quantity allowing us to describe the behavior of electron pairs in microscopic systems. In the past several years it was proven to provide new valuable insights into the role of electron pairing in chemical bonds. Especially useful in this respect were found the approaches known as the analysis of domain averaged Fermi holes (DAFH) and the generalized population analysis (GPA). These approaches have been applied to the elucidation of electron reorganization during the carbocationic rearrangements involved in the biosynthesis of terpenes and important new insights were also obtained from the generalization of the DAFH analysis for the description of the bonding interactions in solids.

[Refs. 1, 8]

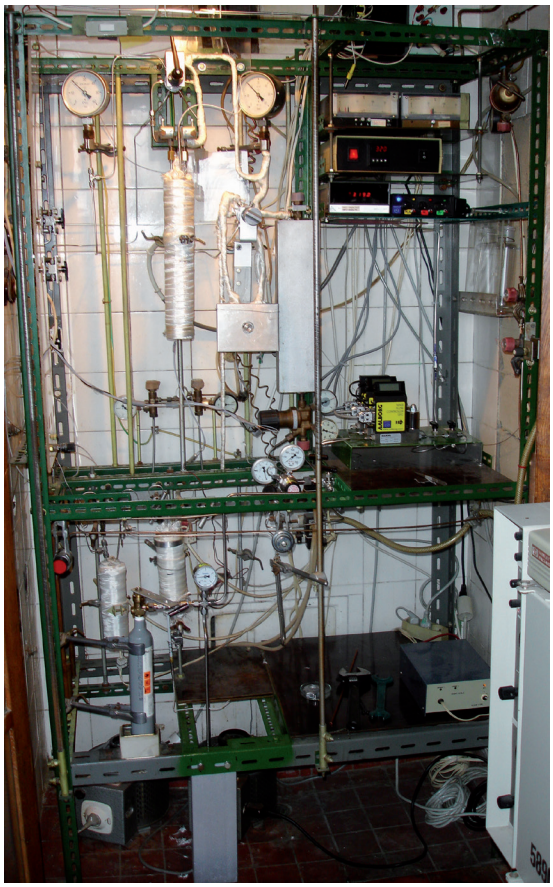


DAFH orbital from the DFT calculation for the cubic hydrogen lattice. The isosurface of the orbital amplitude 0.0107 are colored with the orbital sign. The basin of the corresponding DAFH is located in the middle of the region

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)

Modification of mesoporous silica-alumina by nitric acid extraction was used for preparation of catalysts with a conventional CoMoS phase. Extraction of support significantly increased its BET surface area and protonic acidity, which both positively influenced the hydrodesulfurization (HDS) activity of catalysts. This is because of leaching of non-acidic aluminum oxide which blocks the strong acidic tetrahedral Al-OH-Si sites. Protonic acidity of catalysts was evaluated by means of tests in skeletal isomerization of cyclohexene and cracking of cumene. On the other hand, acid extraction diminished the amount of deposited Mo phase. It was found that the higher dispersion of active phase and specific activities in benzothiophene HDS were achieved on samples synthesized from the modified supports. An interesting point is that the catalysts keep the strong protonic acidity also after deposition of the CoMoS phase.

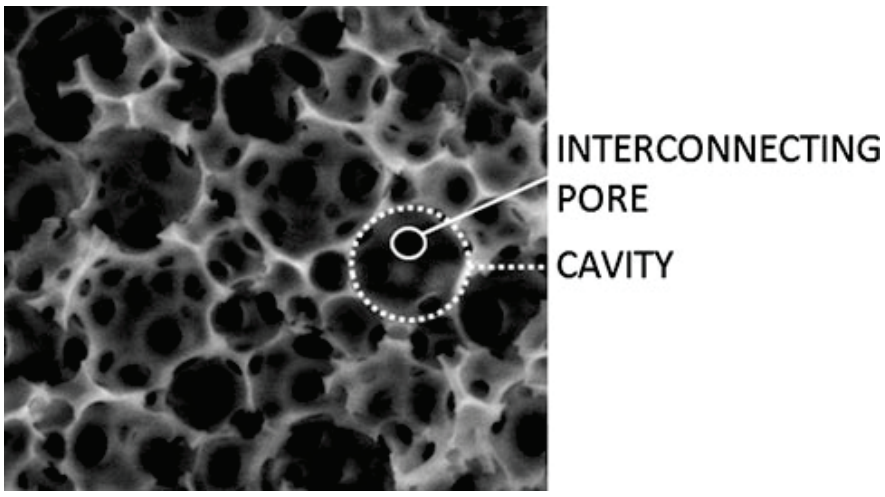


Pressure flow microreactor with fixed bed of catalyst for hydrodesulfurization

Post-polymerization hypercrosslinking of monolithic polymers

(K. Jeřábek, kjer@icpf.cas.cz; joint project with University of Maribor, Slovenia; supported by MEYS, project No. MEB091107)

Within this project are investigating possibilities of modifications of morphology of monolithic PolyHIPE porous polymers by additional crosslinks introduced to the already polymerized monolithic material. In this manner, much smaller pores are created thus significantly enlarging the surface area while leaving the larger pores intact. [Ref. 29]

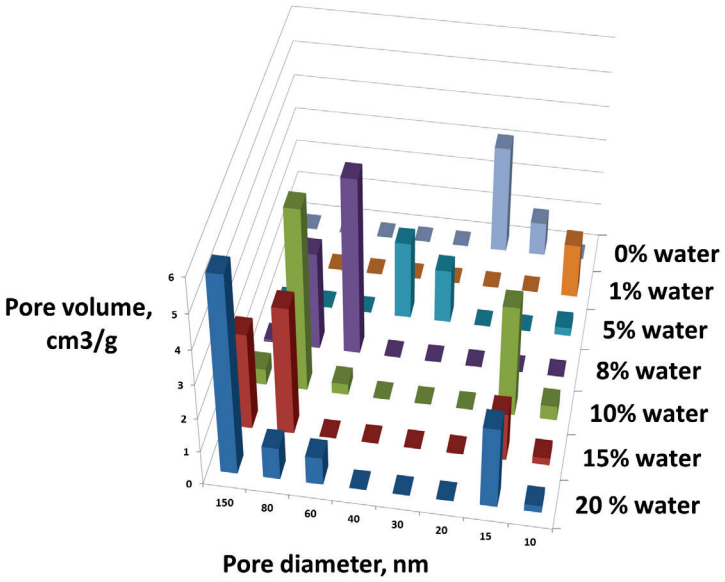


SEM picture showing typical structure of PolyHIPE monolith

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. 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. [Ref. 16]

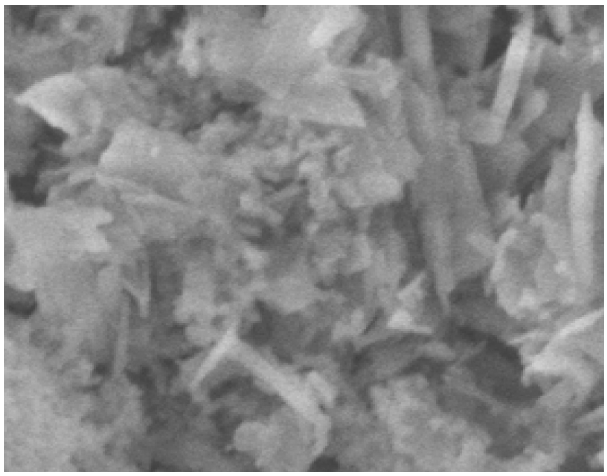


Dependence of swollen-state morphology of poly(divinylbenzenes) on water presence in the porogenic solvent

New catalysts for VOC oxidation

(P. Topka, topka@icpf.cas.cz; joint project with Department of Process and Environmental Engineering, University of Oulu, Finland; supported by ASCR, project No. M200720901)

Commercial VOC oxidation catalysts can be used as comparative materials during development of new or improved catalysts. The objective of this study was to investigate physicochemical properties of EnviCat® commercial catalysts and their performance in total oxidation of three model compounds (dichloromethane, toluene and ethanol) at laboratory scale. The reactivity of model volatile organic compounds was decreasing in the order ethanol > toluene > dichloromethane. The Cu–Mn/Al catalyst was found to be the most active and selective catalyst in ethanol oxidation. In oxidation of dichloromethane, the Pt–Pd/Al–Ce catalyst with 0.10 wt. % Pt + Pd was the most active, while the most selective one (giving the highest HCl yield) was the Pt–Pd/Al catalyst containing 0.24 wt. % Pt + Pd. In toluene oxidation, the Pt–Pd/Al catalyst with 0.24 wt. % Pt + Pd possessed the highest activity; the selectivity to CO_2 was 100 % for all investigated catalysts. Obtained results showed that the performance of commercial catalysts in laboratory scale tests can be different from that declared by catalyst supplier. A possible difference in catalytic performance at industrial and laboratory scale should be taken into account when industrial catalysts are used in laboratory scale tests. [Ref. 25]

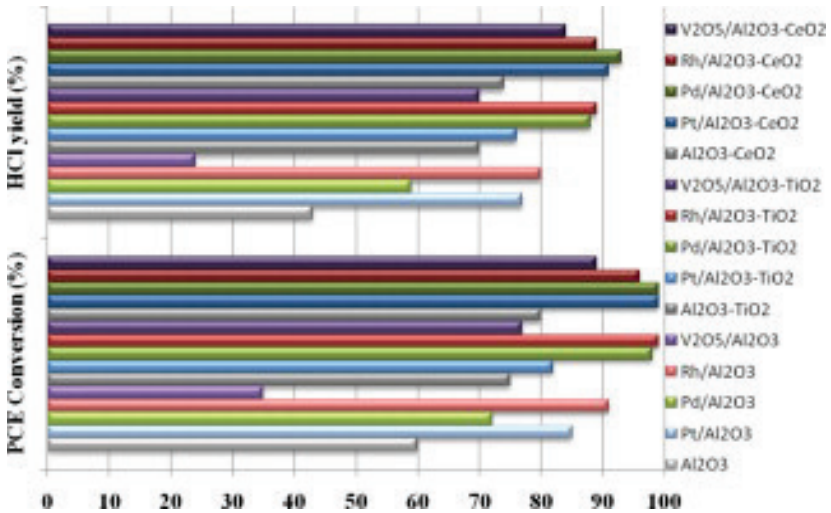


Surface of Envicat® VOC-1544 catalyst as seen by field-emission scanning electron microscope

Development of oxide catalysts for total oxidation of ethanol

(J. Gaálová, gaalova@icpf.cas.cz; supported by GACR, project No. 106/10/P019)

Pt, Pd, Rh and V_2O_5 metallic monolithic catalysts supported on Al_2O_3, Al_2O_3-CeO_2 and Al_2O_3-TiO_2 were examined in the oxidation of perchloroethylene. To ensure high HCl yields, the amount of water as a hydrogen source was optimized to be 1.5 wt. % by testing the effect of water content on perchloroethylene oxidation. Water not only enhanced the selectivity towards HCl formation but also improved the perchloroethylene oxidation to some extent. Both activity and selectivity of the catalysts were found to be related to the properties of the catalyst support; addition of TiO_2 or CeO_2 into Al_2O_3 enhanced catalysts' efficiency regardless of the active phase. Pt, Pd and Rh catalysts showed high catalytic activity, perchloroethylene conversions ranging from 72% to 99%, and HCl yields from 59% up to 93% were observed. Both activity and selectivity of the Pt/Al_2O_3-CeO_2 and Pd/Al_2O_3-CeO_2 catalysts were superior to the other tested catalysts. The results show that in the oxidation of perchloroethylene, the redox properties of the catalyst and the amount of activated oxygen may play bigger role than the acidity. To confirm the suspected positive effect on perchloroethylene oxidation coming from the bidisperzed mesopores seen over ceria-doped catalysts needs further testing. [Refs. 31, 32]

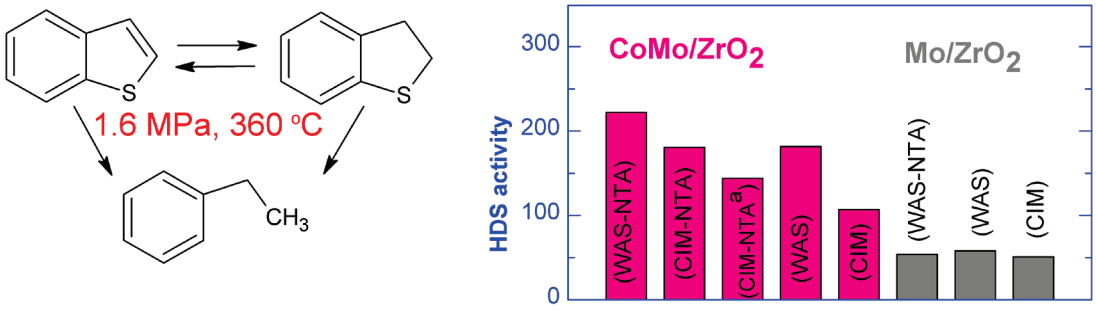


Conversion of perchloroethylene and yield of HCl achieved over investigated catalysts

Unconventional composition and preparation of sulfide hydrotreating catalysts

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

The principles of the use of chelating agents such as nitrilotriacetic acid (NTA) were studied for our original preparation methodology. It was found that the employing of NTA during preparation of CoMo catalysts supported on the monoclinic ZrO_2 increased the hydrodesulfurization (HDS) activity within the range 22–69 %. The molar ratio NTA/(Co+Mo) to achieve high HDS activities was 1/1. The most active CoMo/ZrO_2 catalyst was prepared by the impregnation of the support from the solution made by dissolution of MoO_3, $CoCO_3$ and NTA in water followed by sulfidation without previous calcination. Furthermore, the new alumina-supported NiMo hydrodesulfurization catalysts have been prepared by loading the Anderson-type nickel heteropolyoxomolybdate on the alumina initially modified with nickel, cobalt or boron. Nickel incorporation in the alumina prior to loading (molar ratio of the total amount Ni in the catalysts is Ni/(Mo+Ni) = 0.24) resulted in an activity for 1-benzothiophene HDS that was nearly twice as much as the activity observed for the unmodified, B- and Co modified catalysts. The new mesoporous silica-alumina (SA) was modified by acid leaching and studied as an alternative support for Mo and CoMo catalysts for HDS of benzothiophene, cyclohexene isomerization and cumene cracking. Progressive leaching of the parent SA containing 52 wt. % Al_2O_3 (SA52) led to decrease of Al_2O_3 content (33 and 19 wt. % in MSA33 and MSA19 support, respectively). This decrease was accompanied with an increase of the surface area and exposition of strong acidity. [Refs. 6, 9-11, 28]

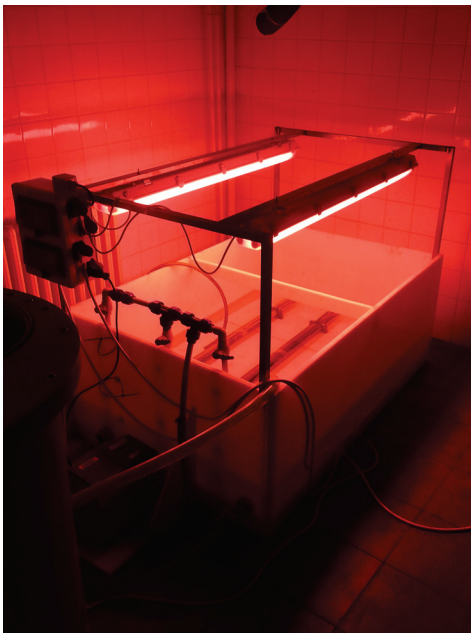


The activity of new CoMo catalysts in hydrodesulfurization of 1-benzothiophene

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, which will be finished in May 2013, is now 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 again 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.

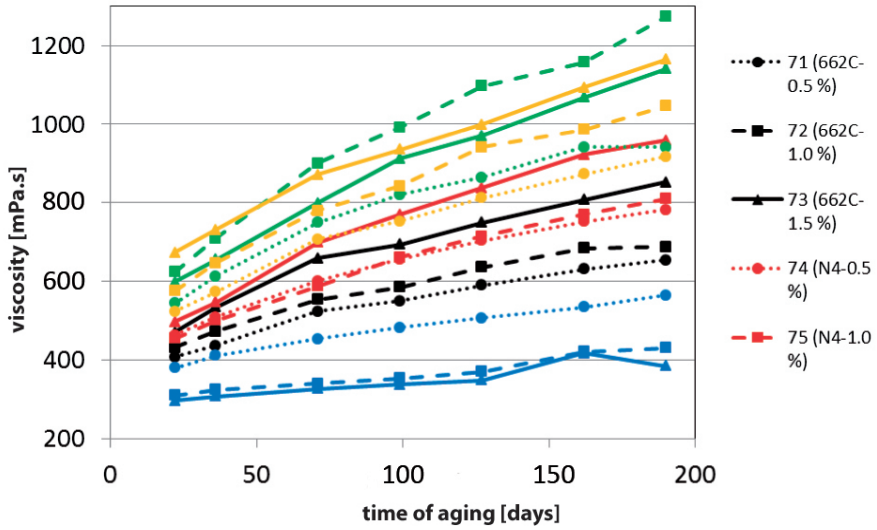


Detail of the phthalocyanine decontamination unit

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 tetraalkylammonium 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)

Composed molecular templates for preparation of assembled functional nanoparticles

(P. Klusoň, kluson@icpf.cas.cz; joint bilateral project with Bangor University, School of Chemistry, Wales, UK; supported by ASCR, project No. M200720904)

This project was finished in March 2012 and t was focusing on making smart functional structures and systems based on template nanoparticles. Among many methods, bottom-up approaches involving templates have dominated for the preparation of one-dimensional or multidimensional nanostructures. This pathway is particularly useful if precise replication is achieved in the nanometer precision. It corresponds to the assembly of well-defined nanobuilding blocks consisting of perfectly calibrated objects keeping their integrity in the final material. In the last project period also ionic liquids were used as molecular patterns and tools for imprinting the structure to the forming nanoparticles. [Refs. 40, 43]

Utilization of combined thermal desorption and catalytic oxidation methods for solid waste decontamination

(O. Šolcová, solcova@icpf.cas.cz; joint project with Dekonta a.s.; supported by MIT, project No. FR-TI1/059)

Project develops and verifies a new technology for decontamination of solid waste containing toxic organic substances, which is based on treatment of the waste by thermal desorption process and subsequent catalytic oxidation of desorbed organic contaminants. Research activities aimed at solution of some technical problems related to full-scale application of the developed technology will be realized together with testing under real conditions.

The combined thermal desorption and catalytic oxidation unit for the soil decontamination was studied at the pilot plant scale. To guarantee flowing of the exhaust gas from the thermal desorption unit into the catalytic oxidation unit the Venturi pump was applied. After the thermal desorption process no residual concentration of contaminants in the soil were detected. Although the contaminant concentrations at the inlet of the catalytic reactor significantly varied during experiments, the efficiency of catalytic oxidation was higher than 90 % in all cases. [Ref. 42]

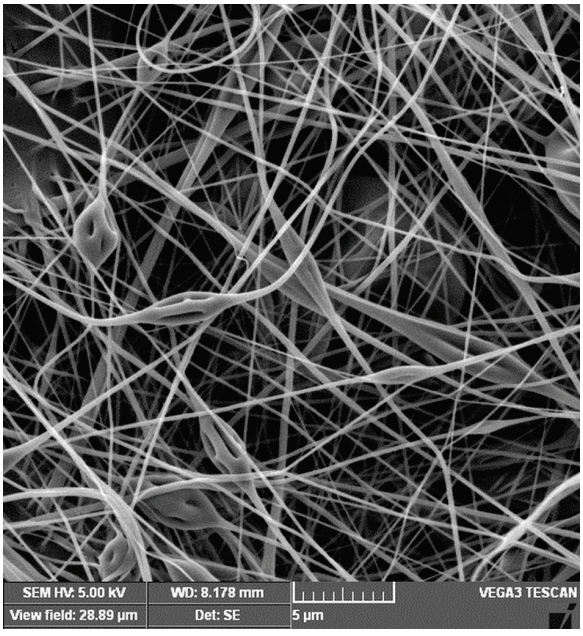
The combined thermal desorption and catalytic oxidation unit

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 science, 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 transport parameters of some porous samples of nanofibrous membranes based on poly(2,6–dimethyl–1,4–phenylene oxide) prepared by electrospinning technology were evaluated. The steady-state counter-current diffusion method was adapted for such type of samples (ultrathin slices of very permeable material, approximately 80% porosity). The special apparatus is able to perform binary diffusion experiments at low-pressure (10–60 kPa). The Knudsen number has a convenient value in this pressure region and the mean free paths of molecules are longer. This fact takes a reasonable effect for transport parameters of macroporous material determination, their precision and confidence. At the same time, the new data evaluating software (boundary value problem connected with parameter optimization by the simplex method) was designed for the transport parameters calculation. Resulting from this approach, the confidence limits for the calculated transport parameters could be determined by the better way. The transport parameter values were compared with their counterparts obtainned by other method – quasi-steady permeation. The steady-state diffusion method processed under low pressure conditions appears as a suitable method for characterization of the quasi-uniform macroporous materials. [Ref. 34]



SEM image of the parent nanofibrous support

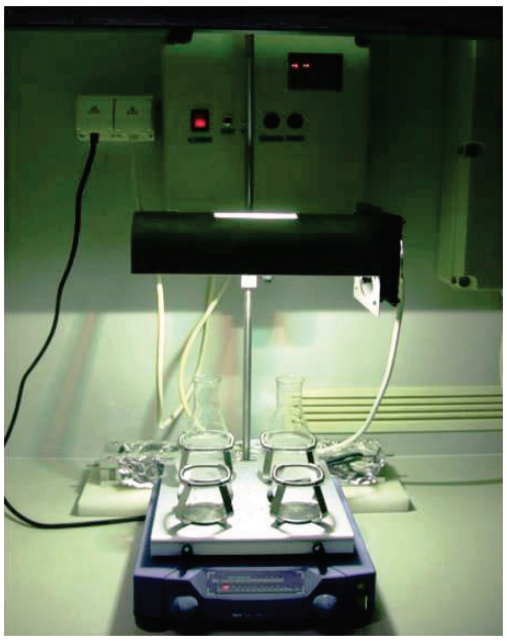
Removal of endocrine disruptors from waste and drinking water by photocatalytic and biological processes

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

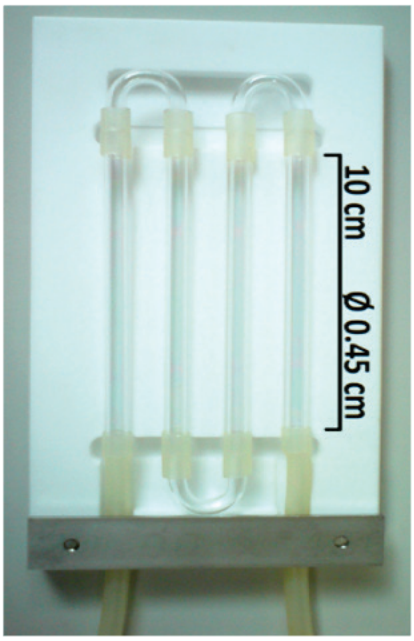
The necessity to find alternative solutions for environmental protection leads to the development and use of the new technologies. Photo-catalysis using semiconductor oxides have found an increasing interest to solve the global pollution problems. Compared to the other photo-catalysts TiO_2 (and/or doped TiO_2) seems to be the most promising material not only in advanced oxidation photo-catalytic processes (AOP). It is well established that titanium oxide and related nanostructure materials in the presence of UV light (in dependence on conditions also in the presence of visible-light) can create very active species that are able to restore and preserve a clean environment by decomposing harmful organics; killing bacteria and viruses and being easily self-cleaned. Our investigation insists on the photo-catalyst immobilization in the form of a thin film trying to improve the efficiency of photocatalytic processes. 17α-ethynylestradiol belongs to the group of the environmental estrogens that act as the hormonal system of the body. Its effect is desirable, especially in hormonal contraception.

The degradation of 17α-ethynylestradiol was measured in the batch and continuous photocatalytic reactors. Initial concentration of ethynylestradiol was in the range 20 to 25 ppm in batch reactor and 11 to 14 ppm in the continuous flow reactor. Four various flow rates (2 ml/min, 1 ml/min, 0.4 ml/min and 0.2 ml/min) were used for degradation of ethynylestradiol in the continuous arrangement. As photocatalyst, TiO_2 thin layers on the glass beads and glass tubes under UV light were applied. 17α-ethynylestradiol degradation activity and selectivity were compared for both arrangements with respect to the possible application.

During the degradation process the estrogenic activity decreased from 97 % to 3 %. Values of the estrogenic activity correspond with decrease of 17α-ethynylestradiol concentration. Conversion of 17-ethynylestradiol (EE2) achieved 94 % after eight hours. No enhanced toxicity was detected during the experiment that stayed at the zero level. [Refs. 14, 15, 18, 26, 35]



Batch photo-reactor



Plug flow microphoto-reactor

Ionic liquids as additives for special pigments

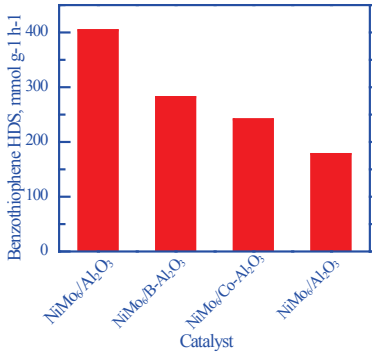
(O. Šolcová, solcova@icpf.cas.cz; joint project with Synthesia, Techem; supported by MIT, project No. FR-TI4/189)

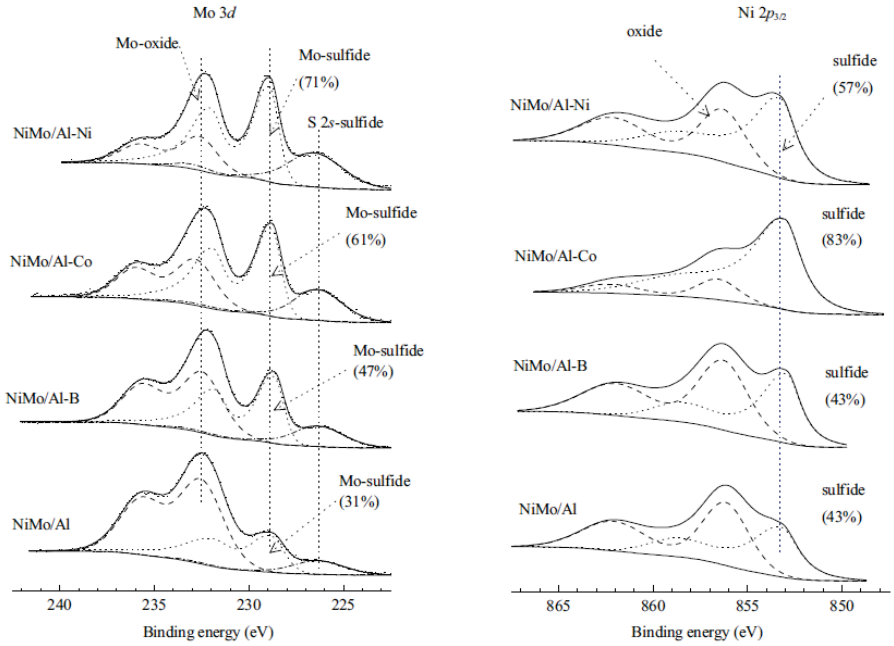
Ionic liquids are composed of large ions with a low degree of the overall molecular symmetry. Very high coloumbic interactions are behind their impressive electrical and mechanical stabilities, thermal and pressure resistivity, and extremely low tension of vapors. Low flammability, very good electrical 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.

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)

A hydrotreating NiMo/γ-Al_2O_3 catalyst (12 wt.% Mo and 1.1 wt. % Ni) was prepared by impregnation of the support with the Anderson-type heteropolyoxomolybdate $(NH_4)_4Ni(OH)_6Mo_6O_{18}$. Before impregnation of the support, it was modified with an aqueous solution of H_3BO_3, $Co(NO_3)_2$, or $Ni(NO_3)_2$. The catalysts were investigated using N_2 adsorption, O_2 chemisorption, X-ray diffraction, UV-Vis spectroscopy, Fourier transform infrared spectroscopy, temperature-programmed reduction, temperature-programmed desorption, and X-ray photoelectron spectroscopy. The addition of Co, Ni, or B influenced the Al_2O_3 phase composition and gave increased catalytic activity for 1-benzothiophene hydrodesulfurization (HDS). X-ray photoelectron spectroscopy confirmed that the prior loading of Ni, Co or B increased the degree of sulfidation of the NiMo/γ-Al_2O_3 catalysts. The highest HDS activity was observed with the NiMo/γ-Al_2O_3 catalyst with prior loaded Ni. TiAlZr mixed oxides, synthesized using sol-gel method, were characterized and used as supports of HDS catalysts prepared by impregnation either with molybdenum heteropolyacid or its cobalt salt. No formation of a new oxide phase was revealed in the synthesized mixed materials. Incorporation of cobalt into the catalyst masked the effect of the support composition. [Refs. 10, 17, 28]



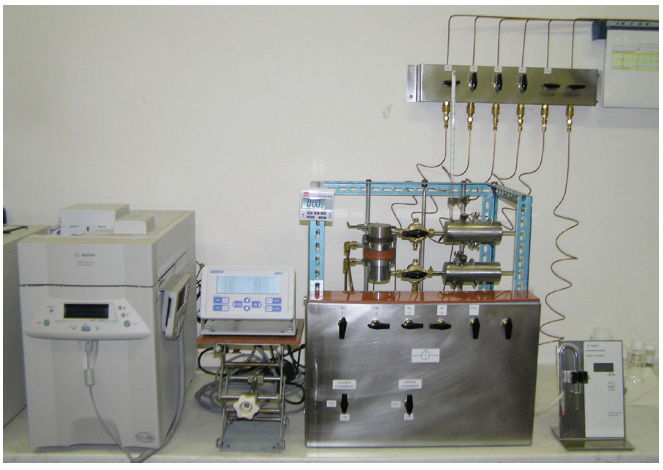


The preparation of CoMo catalysts using Anderson-type heteropolyoxomolybdate: effect of Al_2O_3 modification on benzothiophene HDS and XPS patterns

Transport characteristics of novel biocompatible materials

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

The development and design of advanced bioactive and biocompatible porous materials for medical applications requires a thorough understanding of the texture and transport properties impact on their clinical efficiency. The project is focused on mass transport measurements and the transport characteristic determination of biocompatible clinical valuable materials consisted of nanofibrous mats/membranes prepared by electrospinning technique, hydroxyapatite and apatite. Transport characteristics are determined in liquid/solid as well as gas/solid systems by combination of inverse liquid chromatography and Graham's diffusion cell methods. Effective diffusion coefficients in liquid phase are evaluated using a method based on the fitting of a set of experimental chromatographic profiles to the Kubín-Kučera model. Fitting of the gas diffusion data obtained from Graham's diffusion cell to the Mean Transport-Pore Model provide transport characteristics. The obtained transport parameters are compared with characteristics from the standard textural analyses. [Ref. 33]

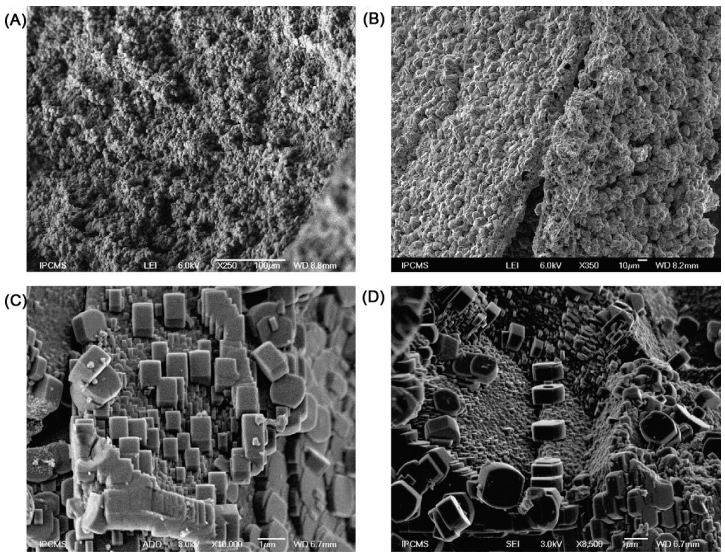


Graham's diffusion cell setup

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). In order to prepare material with the strict hierarchical pore structure it is the key factor to know both the transport and texture characteristics typical of its pore network. Pore structure depends not only on chemical composition, but also on the preparation method and has, therefore, to be determined experimentally. Experimental setups based on the inverse gas chromatography method (the Single Pellet String Column arrangement of the chromatography column) together with Graham's diffusion cell apparatus are utilized for the obtaining transport characteristics of tested ordered materials.

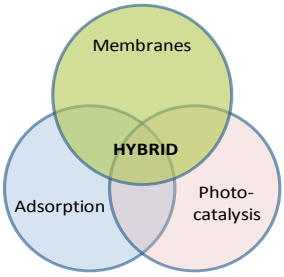


SEM micrographs of ZSM-5 zeolite coated on β-SiC foam (A, B, C and D)

Hybride membrane process for water treatment (HYMEPRO)

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

Project deals with the development of a novel, active and sustainable hybrid wastewater treatment process that removes simultaneously heavy metals, arsenic and nutrients from waters. The developed technology is designed based on the green chemistry and engineering principles. [Refs. 23-25, 31, 32]



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

(O. Šolcová, solcova@icpf.cas.cz; joint project with EcoFuel Laboratories, s.r.o., 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 for3rd generation of biodiesel production.

Scenedesmus obliquus

Biorefinery research centre of competence - BIORAF

(O. Šolcová, solcova@icpf.cas.cz; joint project with ICT, IBOT, Rabbit Trhový Štěpánov, a.s., Agra group, a.s., Briklis, s.r.o. and EcoFuel Laboratories, s.r.o.; supported by TACR, Competence Centres, project No. TE01020080)

The project 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.).

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.

Helinathus uberosus

Inulin syrup

Photo-bio-reactor

Crude microalgae oil

International co-operations

University of Ghent, Ghent, Belgium: Theory of chemical bond, theoretical characterization of aromaticity
University of Ghent, Ghent, Belgium: Generalized population analysis, theoretical characterization of aromaticity, molecular basis of structure activity relationships
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
University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix
Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Visualization of bonding interactions in transition metal complexes
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
University of Kragujevac, Serbia: Multicenter bonding, quantitative characterization of aromaticity
Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia: Morphology of PolyHIPE materials
University of Barcelona, Barcelona, Spain: Ion exchanger catalysts
Zhejiang University, Hangzhou, China: Mesoporous poly(divinylbenzenes)

University of Vigo, Vigo, Spain: Multicenter bonding, theoretical characterization of aromaticity
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
University of Liverpool, Liverpool, United Kingdom: Theory of chemical bond
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
Department of Physical chemistry, Slovak Technical University Bratislava, Slovakia: visualization of bonding interactions in transition metal complexes
Chemistry department, University of Pecs, Hungary: visualization of the bonding interactions in transition metal complexes
Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany: bonding in solids
Department of Chemistry, University of California-Davis, USA: electron reorganization in carbocationic rearrangements
Istanbul Technical University, Istanbul, Turkey: Synthesis and Thorough Characterization of Composite Functionalized Polymeric Nano-Structure

Visitors

L. Benoit, University of Strasbourg, France
M. Boltz, University of Strasbourg, France
D. Cooper, University of Liverpool, United Kingdom
B. Corain, University of Padua, Italy
J. Grabowski, Central Mining Institute, Katowice, Poland
M. Green, UCG Engineering Ltd, United Kingdom
P. Krajnc, University of Maribor, Slovenia
A. Lobnik, University of Maribor, Maribor, Slovenia
M. Pankiewicz, Central Mining Institute, Katowice, Poland
J. Rogut, Central Mining Institute, Katowice, Poland
A. Sezai Sarac, Istanbul Technical University Faculty of Sciences
A. Spojakina, Institute of Catalysis, BAS, Sofia, Bulgaria
K. Stanczyk, Central Mining Institute, Katowice, Poland
Y. Zub, Institute of Surface Chemistry NAS, Ukraine

Teaching

K. Jeřábek: visiting professor at Polymer Technology College, Slovenj Gradec, Slovenia, course "Functional polymers –morphology and application properties"
P. Klusoň: UJEP, course "Toxicology"
R. Ponec: CU, course "Structure and reactivity"
O. Šolcová: ICT, postgraduate course "Texture of porous solids"

Publications

Original papers

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Department of Multiphase Reactors

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LAB TECHNICIANS
STANISLAVA NOVÁKOVÁ

Fields of research

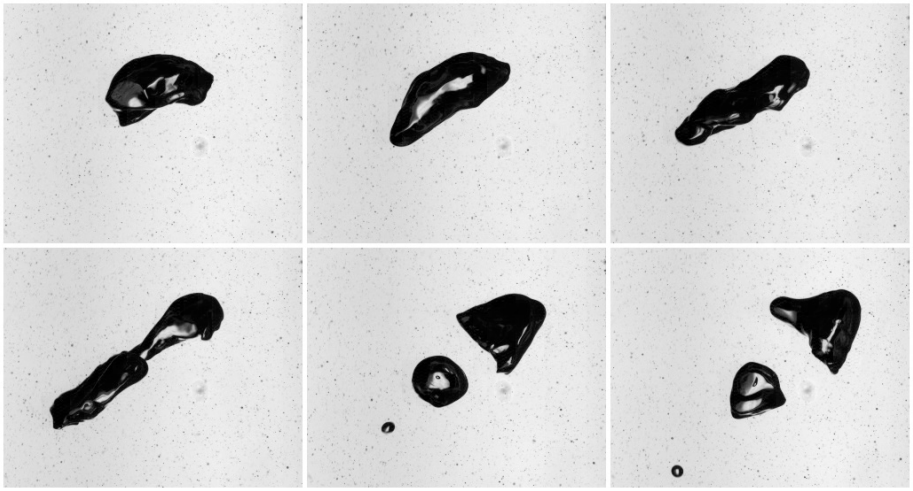
- Multiphase fluid dynamics and transport phenomena in different types of gas-liquid, liquid-solid or gas-liquid-solid systems
- Numerical simulations of transport in complex multiphase systems
- Influence of surface active agents on the multiphase flows
- Flow of microdispersions and liquids with complex rheological behavior
- Electrodiffusion diagnostics of the flow in microfluidic systems
- Flow characterization in fuel cells
- Hydroacoustic aspects of bubbles in natural environment
- Hydrodynamic concept of stromatactis formation in geology
- 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, 7]

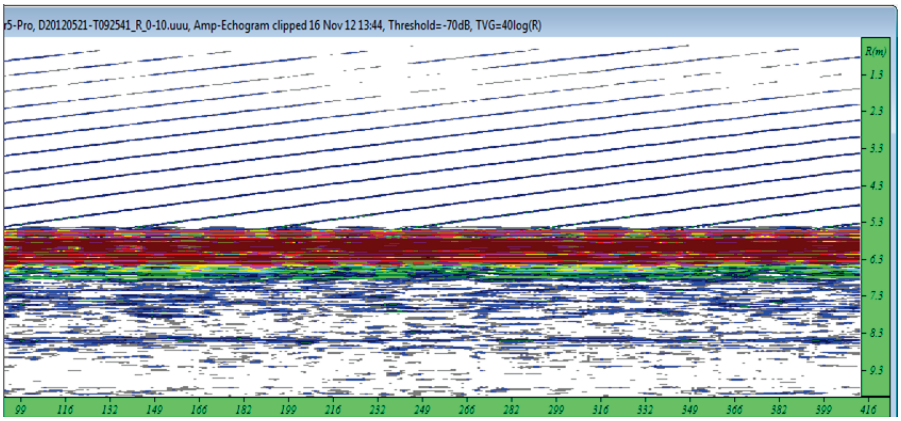


Break-up of a 5 mm bubble in a turbulent flow (interval between frames 12 ms)

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, Biology Centre of the ASCR, v. v. i.; 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.



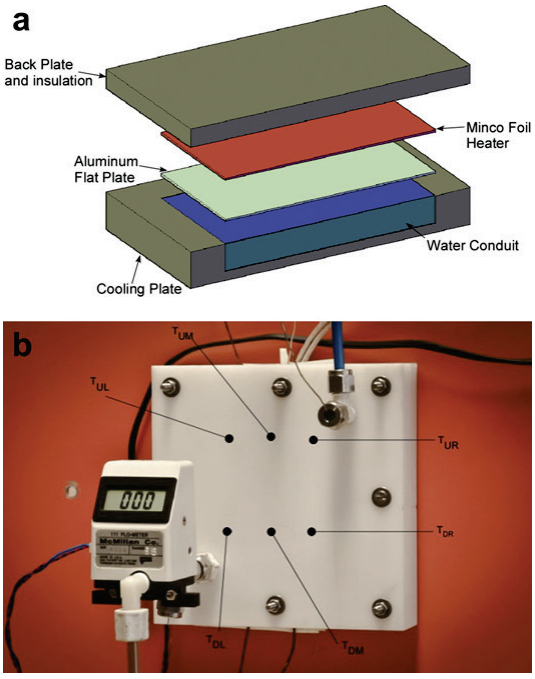
Acoustic echoes of 3 mm bubbles acquired by vertical 120 kHz sonar. Blue lines represent rising bubbles and brown bar represents bottom of the lake (ordinate – water depth, abscissa – time scale in signal pings)

Optimal heat integration of fuel cell systems

(J. Tihon, tihon@icpf.cas.cz; joint project with Aristotle University of Thessaloniki, Greece; supported by MEYS, FP7, 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.

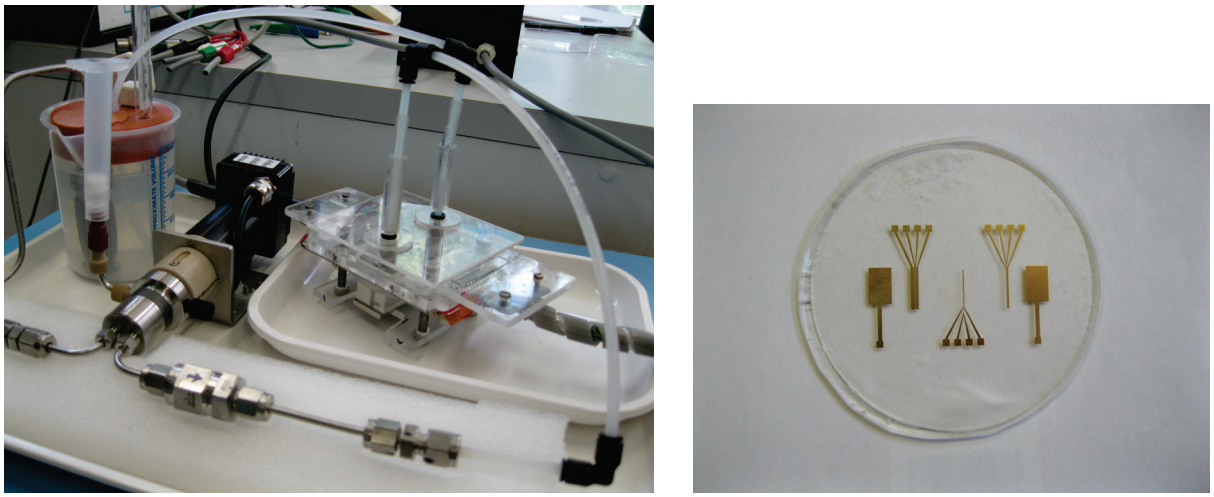


The experimental unit for the study of thermal behavior of the PEM fuel cells in Thessaloniki: (a) schematic representation, (b) photograph with the marked positions of thermocouples

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. 6]

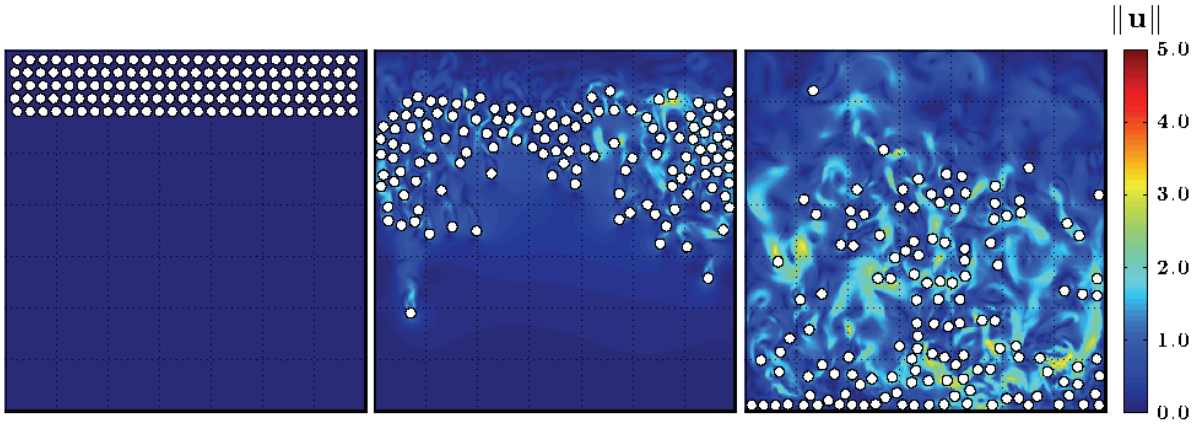


Experimental set-up used for electrodiffusion diagnostics of the flow in microchannels (left) and shown in detail the chip with microsensors (right)

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.

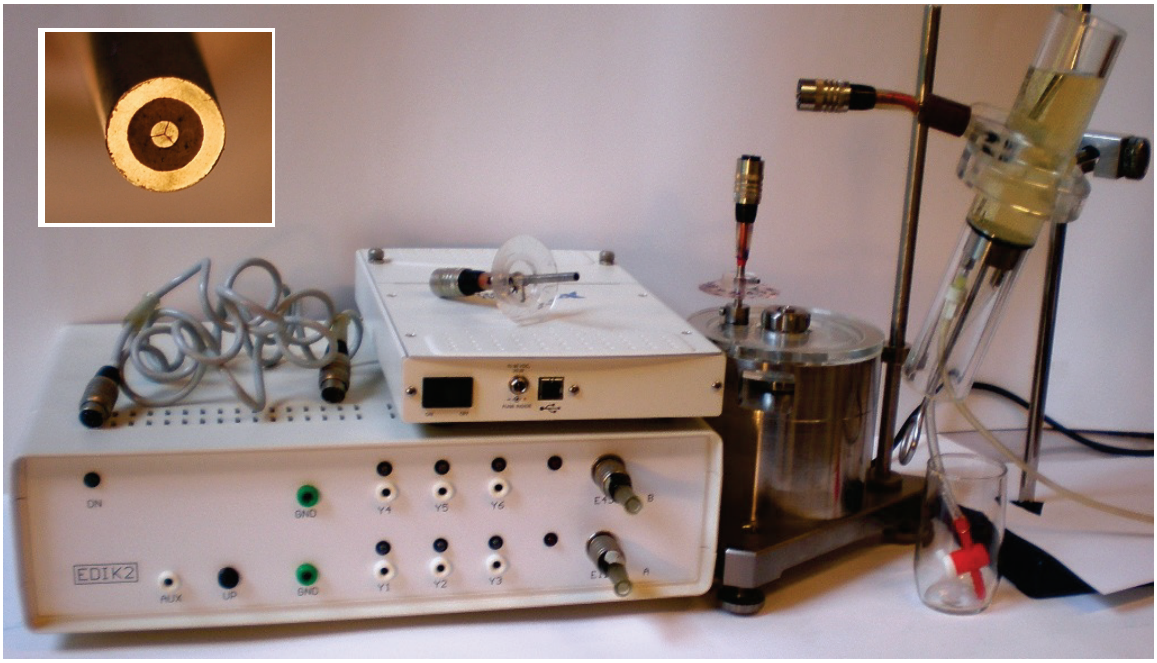


Sedimentation of 135 rigid particles simulated with immersed boundary method

Estimate of mass transfer rate via Nernst model with ohmic losses

(O. Wein, weinbrevnov@seznam.cz; supported by GACR, project No. 104/08/0428)

The liming current technique, employed e.g. in electrodiffusion flow diagnostics, is based on an oversimplified electrochemical concept, which accounts only for the convective transport of depolarizers across a diffusion layer with constant bulk and wall concentrations. However, there are additional transport resistances that cannot be neglected: Faradaic resistance at surface of working electrode, and Ohmic losses in the bulk of electrolyte solution. Effect of these additional resistances is analyzed using the Nernst model of a two electrode cell (no reference electrode). The Faradaic resistances due to electrode kinetics are considered for a single redox couple O + *n*e = R according to the Butler-Volmer electrode kinetics. The effect of Ohmic losses is accounted for, considering primary current distribution for a uniformly accessible circular electrode. [Ref. 8]

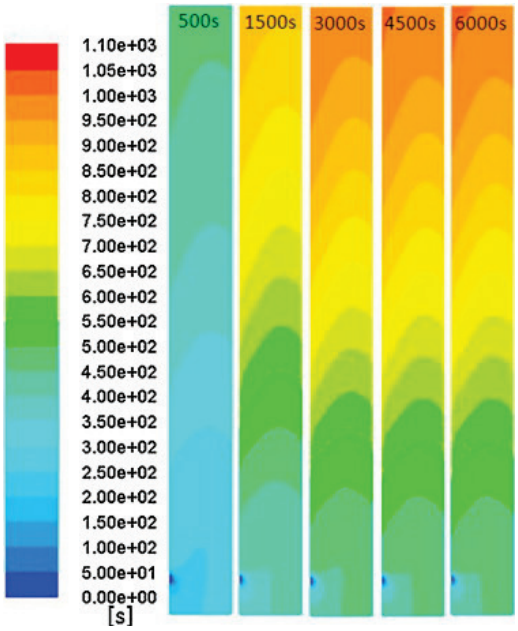


Setup for electrodiffusion experiments, used here in a voltamperometric study with three-segment electrodes

Smart RTD (residence time distribution) for multiphase flow systems

(M. Šimčík, simcik@icpf.cas.cz, cooperation with University of Minho, Braga, Portugal)

A relatively new concept is presented for evaluation of the fluid age distribution within the interior of an apparatus. In the standard RTD approach, the tracer study is performed and RTD is obtained. In the new approach denoted as SRTD, the fluid age is considered as the field quantity and the governing equation is formulated for its spatio-temporal distribution within the flow domain. There are only few studies devoted to this alternative approach, which typically concern only the single-phase flow systems. In this contribution we investigate its applicability also to multiphase systems. In the case of a bubble column, both the RTD and SRTD concepts are employed and discussed. The results are calculated numerically and compared with the experimental observations. [Ref. 5]



Patterns of the spatio-temporal dynamics of the liquid age distribution in a bubble column. Shown in the domain symmetry plane for Q_L = 80 l/h

Hydrodynamic concept of stromatactis formation in geology

(M. Růžička, ruzicka@icpf.cas.cz; joint project with Institute of Geology of the ASCR, v.v.i.;
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. The interdisciplinary study is novel, and the results are fundamental for sedimentology and hydrodynamics, with possible implications in related technologies.

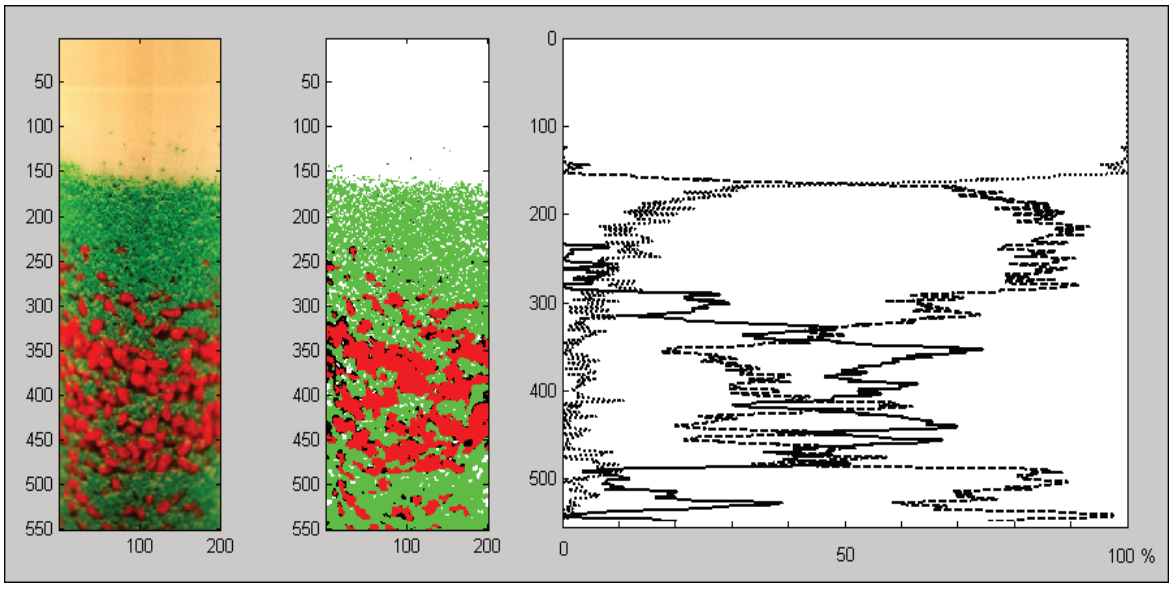


Image analysis of the deposit pictures. The photo (left) was converted into binary numbers (middle) from which was calculated distribution of particle fractions along the deposit height (right). Abscissa - percentage of individual size fractions of particles, ordinate - deposit height; the largest size fraction (red) - full line, middle size fraction (green) - dashed, the smallest size fraction (white) - dotted

International co-operations

Berlin Institute of Technology, Germany: Multiphase flow diagnostics
CRTT, Saint Nazaire, France: Microfluidics
Institute of Fluid Mechanics, Toulouse, France: Effect of surfactants on multiphase flows
University of Valenciennes, France: Electrodiffusion diagnostics of the flow
Aristotle University of Thessaloniki, Thessaloniki, Greece: microfluidics
Norwegian Institute of Technology (NTH), SINTEF, Trondheim, Norway: Bubble columns
University of Minho, Braga, Portugal: Multiphase bubble bed reactors

Visitors

S. Grillo, Universita degli Studi di Napoli Federico II., Italy (Erasmus)
Q. Mouret, ENSEEIHT Toulouse, France (Erasmus)
N. Begue, INP Toulouse - ENSIACET, France (Erasmus)
A. Lemarchand, INP Toulouse - ENSIACET, France (Erasmus)
A. Rollin, INP Toulouse - ENSIACET, France (Erasmus)

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 Simulation of Transport Process"
J. Tihon, J. Vejražka: ICT, Faculty of Chemical Engineering, postgraduate course "Bubbles, drops, and particles"

Visits abroad

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

Publications

Original papers

[1] Abi Chebel N., Vejražka J., Masbernat O., Risso F.: Shape Oscillations of an Oil Drop Rising in Water : Effect of Surface Contamination. *J. Fluid Mech.* 702, 533-542 (2012).

[2] Izák P., Kárászová M., Vejražka J., Friess K., Randová A., Jansen J.C.: The Effective Upgrading of Raw Biogas to Methane by Selective Membranes. *Procedia Eng.* 44, 429-431 (2012).

[3] Kárászová M., Vejražka J., Veselý V., Friess K., Randová A., Hejtmánek V., Brabec L., Izák P.: A Water-Swollen Thin Film Composite Membrane for Effective Upgrading of Raw Biogass by Methane. *Sep. Purif. Technol.* 89, 212-216 (2012).

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[5] Šimčík M., Růžička M., Mota A., Teixeira J.A.: Smart RTD for Multiphase Flow Systems. *Chem. Eng. Res. Des.* 90(11), 1739-1749 (2012).

[6] Tihon J., Pěnkavová V., Havlica J., Šimčík M.: The Transitional Backward-Facing Step Flow in a Water Channel with Variable Expansion Geometry. *Exp. Therm. Fluid Sci.* 40, 112-125 (2012).

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[8] Wein O.: Estimate of Mass-Transfer Rate via Nernst Model with Ohmic Losses. *Russ. J. Electrochem.* [*Elektrokhimiya* 48(7), 778-785 (2012)] 48(7), 704-711 (2012).

Patents

[9] Hájek M., Sobek J., Brustman J., Veselý V., Drahoš J.: Method for the Chemical Depolymerization of Waste Polyethylene Terephthalate. Pat. No. CN101688015/200880002443.4. Applied: 10.01.12, patented: 12.09.19.

[10] Izák P., Kárászová M., Vejražka J.: Způsob separace plynné směsi a zařízení k provádění tohoto způsobu. (Czech) A Process for the Separation of a Gaseous Mixture and an Apparatus for Carrying Out the Same. Pat. No. CZ303107/PV 2010-438. Applied: 11.06.20, patented: 12.04.04.

[11] Izák P., Poloncarzová M., Vejražka J.: Způsob obohacení bioplynu z čističek odpadních vod nebo zemědělské prvovýroby o methan a zařízení k jeho obohacení. (Czech) The Method and the Apparatus for Methane Enrichment of Biogas from Sewage Plant and Agriculture. Pat. No. CZ303106/PV 2010-437. Applied: 10.06.02, patented: 12.02.23.

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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
- Structure of silyl moieties through $J(^{29}Si\text{-}^{13}C)$ couplings as determined by triple $\{^{1}H, ^{13}C\}^{29}Si$ NMR experiment
- 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

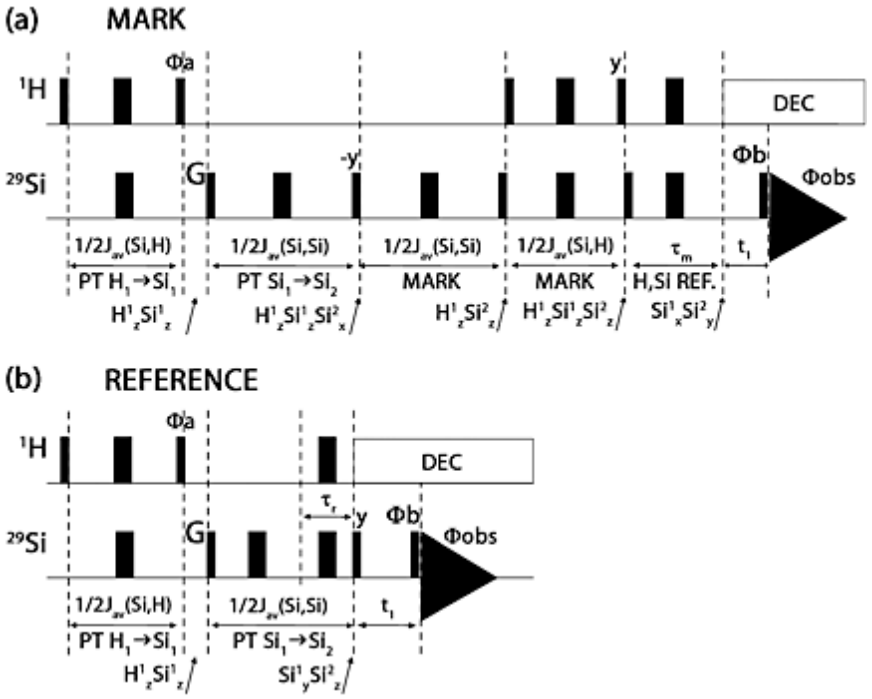
- Enzymatically catalyzed synthesis of alkyd resins
- Development of new analytical methods
- Analytical services to the research departments of ICPF
- Multigram scale production of helicenes and [*n*]phenacenes

Research projects

Spectra edited by relative signs of homonuclear couplings of low abundance nuclei

(V. Blechta, blechta@icpf.cas.cz; supported by GA AVCR, project No. IAA400720706, and GACR, project No. 203/08/P412)

The proposed homonuclear coupling sign edited (HCSE) experiment can detect signed homonuclear couplings between low abundant nuclei like ^{13}C, ^{29}Si and ^{15}N in linear spin systems, that is, in systems where two nuclei are coupled by the measured coupling, and one of them is coupled by a second coupling to a nucleus of different kind. The third nucleus is usually high abundant hydrogen. Two spectra are measured during the HCSE experiment. Their weighed sum and difference yield two other spectra, one containing peaks coupled only by positive measured couplings and the other having peaks coupled by negative measured couplings. The usual E-COSY-type experiment requires all three couplings in the three spin system (triangular spin system) and not only two couplings as the HCSE experiment. The experiment was successfully tested on known carbon–carbon and silicon–silicon two bond couplings. A set of six simple siloxanes with ^{2}J(Si-O-Si) couplings ranging from 0.5 to 9.0 Hz was measured for the first time, and all the couplings were found to be positive. [Ref. 1]



Scheme of HCSE experiment with silicon–silicon coupling detection

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

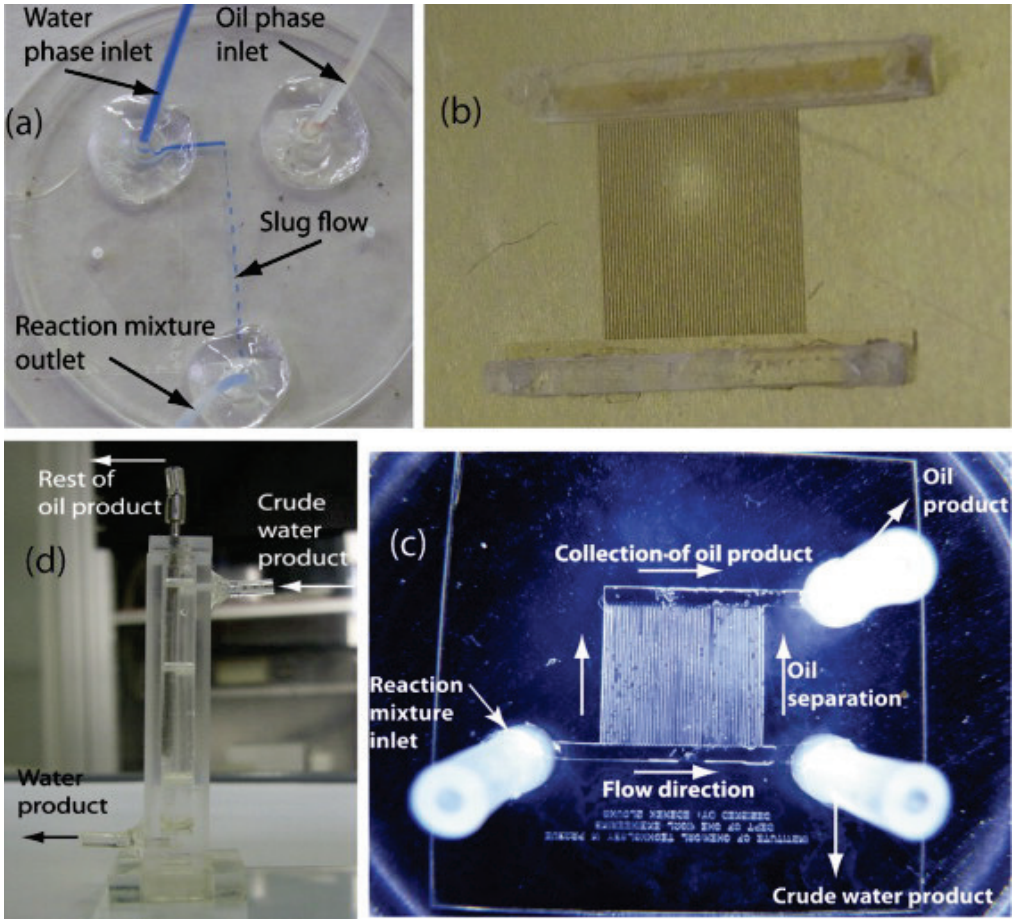
(G. Kuncová, kuncova@icpf.cas.cz; supported by MEYS, ESF, project No. CZ.1.07/2.3.00/20.0092)

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).

Enzyme hydrolysis of soybean oil in a slug flow microsystem

(G. Kuncová, kuncova@icpf.cas.cz; joint project with ICT and University of Notre Dame, USA; supported by MEYS, KONTAKT ME892, project No. MSM6046137306)

We report on the development of a continuous microfluidic reaction system for hydrolysis of soybean oil catalyzed with *Thermomyces lanuginosus* lipase (Lipolase 100 L). The microfluidic reaction system generates water–oil emulsions in the form of a hydrodynamically well controlled slug flow and automatically separates the oil phase after the hydrolysis by employing two microfluidic separators. All elements of this reaction system were tested at different hydrodynamic conditions and showed the ability to operate in a wide range of reactant flow rates. 25–30% conversion of triglyceride was reached in setting the residence time of the emulsion mixture to 10 min. This conversion increased to almost 50% for the residence time of 1 h. These results are comparable with those published for the same enzyme reaction system. This feature along with the benefits stemming from the use of microfluidics make our developed system a useful, easy to control and easy to scale-up technology for fast production of fine chemicals. Moreover, our calculations indicate that our slug flow system allows for significant savings of the mechanical energy. [Ref. 3]



(a) Microfluidic generator of the slug flow. Blue water solution is introduced in one microchannel for the interface contrast enhancement, (b) primary microseparator – SU8 master on phosphorbronze substrate, (c) primary microseparator – PDMS microchip, and (d) secondary microseparator

Preparation of helicene based chiral stationary phase for HPLC

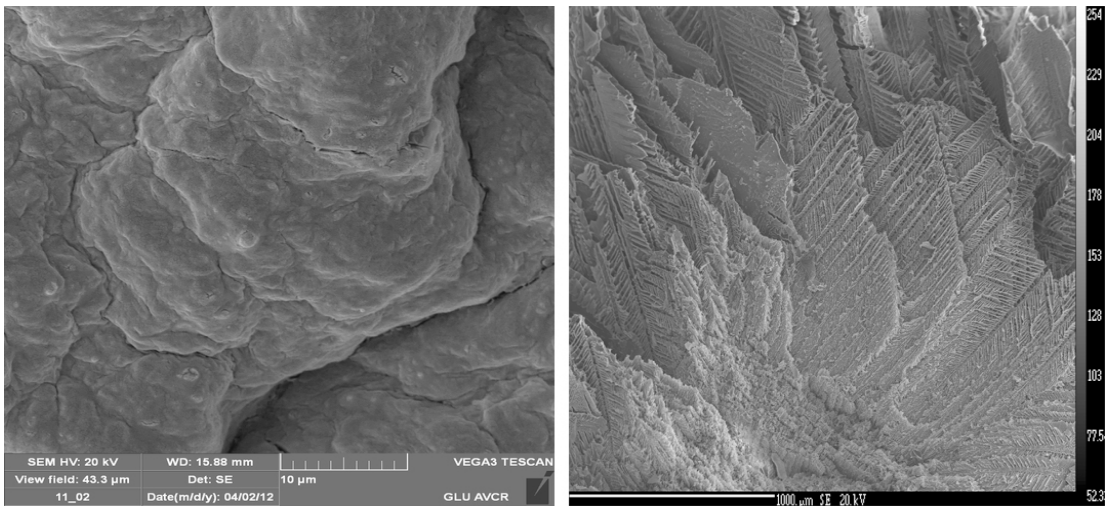
(J. Sýkora, sykora@icpf.cas.cz; joint project with Watrex Praha, s.r.o.; supported by TACR, project No. TA01010646)

The main aim of the project is to develop a new stationary phase for HPLC which would serve for column manufacturing. Further testing of its properties and evaluation of the relevancy for possible production and sale is also part of the objectives. [Ref. 15]

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 (A) and 92% for biocatalyst frozen in liquid nitrogen (B).

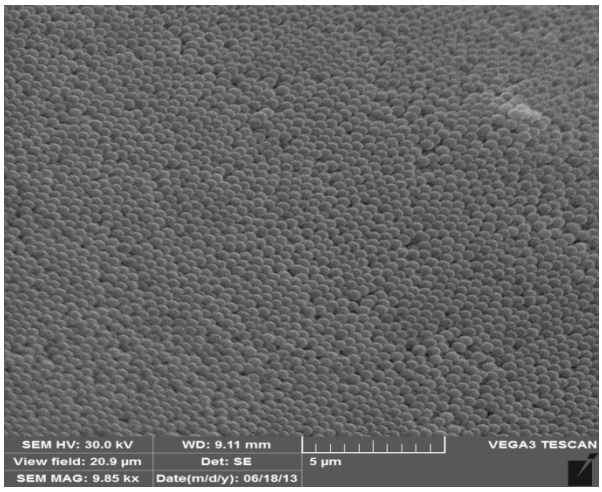


Structure of lipase – montmorillonite biocatalyst (A)- dried at ambient temperature (B) – frozen in liquid nitrogen (ISISA)

Calixarene-porphyrin conjugates for selective complexation and separation of fullerenes

(S. Šabata, sabata@icpf.cas.cz; joint project with ICT and IIC; supported by GACR, project No. 203/09/0691)

The silanized tetraamoniumporphyrine, which we had synthetized in 2010, was chemically bounded on surfaces of inorganic materials; montmorillonite and various silica nanoparticles. Commercially available LUDOX and monodisperze spherical silica particles prepared by modified Ströber method were used. These composite materials comprising silanized tetraamoniumporphyrine were mixed with tetraethoxysilane and filled into empty chromatography columns (Ø 4 mm, length 150 mm). After gelation, interconnected hierarchical micro-/meso-/macroporous networks were created by ice segregation induced self-assembly method. Such monolithical chromatography columns performed low separation abilities due to presence of large pores.

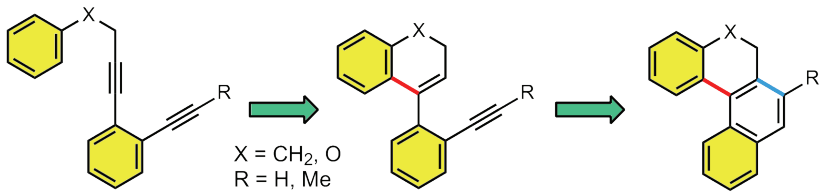


Monodisperze spherical silica particles with chemically bounded silanized tetraamoniumporphyrine

Synthesis of helicenes *via* cycloisomerization of biphenylylnaphthalene and 1,8-diarylnaphthalene derivatives

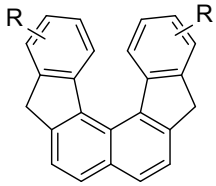
(J. Čermák, J. Storch, cermak@icpf.cas.cz, storchj@icpf.cas.cz; supported by GACR, project No. 207/10/1124)

The new $PtCl_2/PtCl_4$ catalyzed hydroarylation / cycloisomerization cascade reaction leading to formation of two aromatic or heteroaromatic rings in one step is reported. The strategy developed is exemplified by the synthesis of 5,6-dihydrobenzo[*c*]phenanthrene and 6*H*-naphtho[2,1-*c*]chromene skeletons. Attempts to [8]helicene-like molecules were also investigated. The results were published in *Eur. J. Org. Chem.* **2013**, *2*, 260-263.



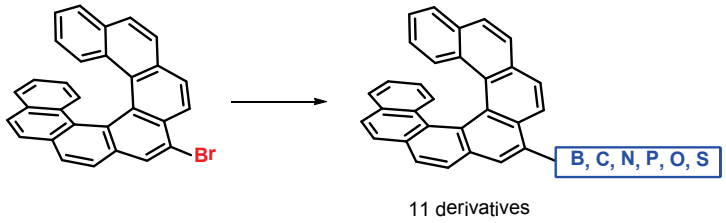
Hydroarylation / cycloisomerization cascade reaction

The synthesis of [6]helicene-like molecules - *pseudo*-helicenes was also developed. Incorporated pyridine rings or diamino derivatives, phosphines and/or diphosphines could find use in coordination chemistry, e.g. as ligands in metal catalysis and organocatalysis. Deprotonated form with cyclopentadienyl ring stabilized with metals (ferocene-like structures) could exhibit increased racemization barrier and thus be applicable in asymmetric reactions. Results on synthesis of model compounds will be published soon.



Exploration of 9-bromo[7]helicene reactivity mainly in Pd-catalyzed reactions is reported. Palladium catalyzed carbon – carbon and carbon – heteroatom coupling reactions provide a large portfolio of racemic helicenes bearing different functional groups in good to excellent yields. Many of the reactions were performed in the microwave reactor saving reaction time to

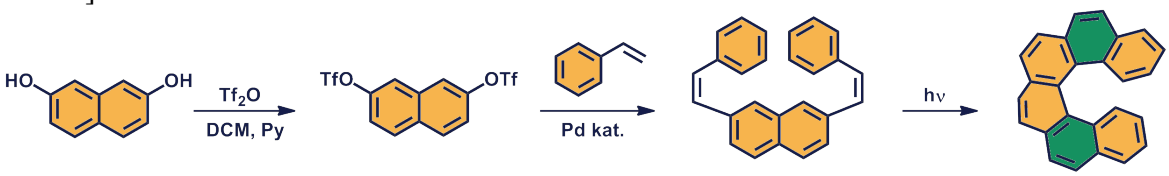
a minimum comparing with conventional and known synthetic methods. These results were submitted in December to *Tetrahedron* **2013**, *69*, 6213-6218.



9-bromo[7]helicene reactivity

Technology of the oxidative photocyclization leading to helicenes (J. Storch, storchj@icpf.cas.cz; supported by MIT, project No. FR-TI3/628)

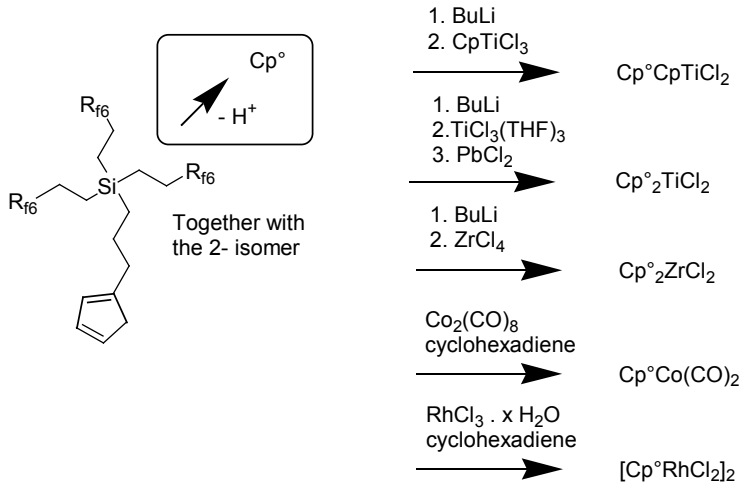
The project is aimed at development of photocyclization apparatus enabling multigram-scale production of various helicenes for distribution in the Czech Republic and abroad. The technology makes exploitation of helicenes in various areas such as separation techniques, supramolecular chemistry, catalysis etc. possible. Intellectual property produced within this project concerning to method and apparatus for production of [6]helicenes was also patented. [Ref. 15]



Synthesis of [6]Helicene from 2,7-dihydroxynaphthalene

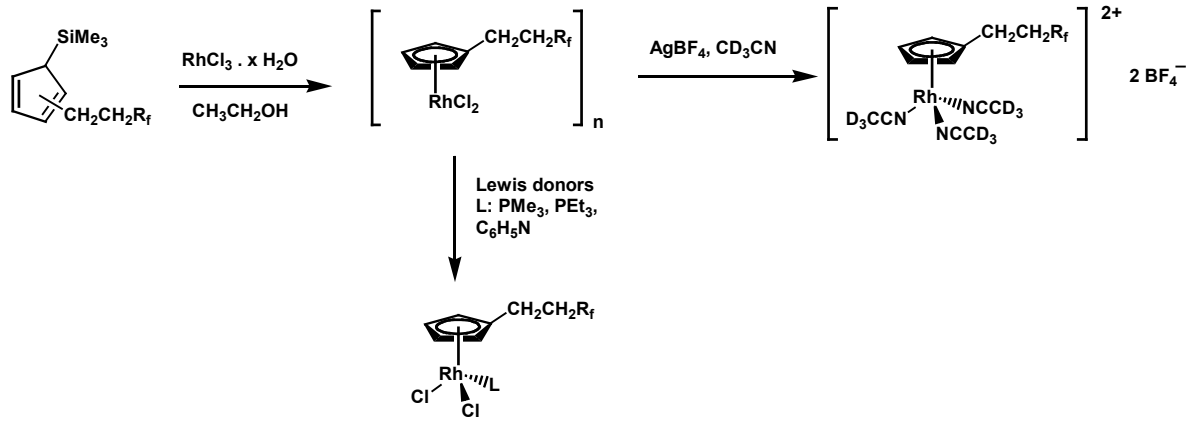
Highly fluorous cyclopentadienes for applications in catalysis
(J Čermák, cermak@icpf.cas.cz; supported by GACR, project No. P106/12/1372)

Two new approaches to synthesis of heavy fluorous (i.e. showing high fluorophilicity) cyclopentadienes and cyclopentadienyl ligands were studied. In the first approach silicon is used as a branching atom and three (perfluoroalkyl)ethyl substituents are attached to it. The whole fluorous tag could be used for fluorophilization of cyclopentadienes. Other nucleophilic substitution reactions provided various functional groups in the core of the tag.



Tagged cyclopentadiene and its reactions

The other approach uses stepwise alkylation of trimethylsilylcyclopentadiene to provide cyclopentadienes polyalkylated with (perfluoroalkyl)ethyl groups. Rhodium complexes of the monosubstituted cyclopentadienyl ligand were prepared and characterized by NMR.



Rhodium complexes with (perfluoroalkyl)ethyl substituent

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

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., Kurfürst M., Schraml J.: Spectra Edited by Relative Signs of Homonuclear Couplings of Low Abundant Nuclei. *Magn. Reson. Chem.* 50(2), 135-141 (2012).

[2] Blechta V., Šabata S., Sýkora J., Hetflejš J., Soukupová L., Schraml J.: The Effect of Solvent Accessible Surface on Hammett-Type Dependencies of Infinite Dilution ^{29}Si and ^{13}C NMR Shifts in Ring Substituted Silylated Phenols Dissolved in Chloroform and Acetone. *Magn. Reson. Chem.* 50(2), 128-134 (2012).

[3] Čech J., Schrott W., Slouka Z., Přibyl M., Brož M., Kuncová G., Šnita D.: Enzyme Hydrolysis of Soybean Oil in a Slug Flow Microsystem. *Biochem. Eng. J.* 67, 194-202 (2012).

[4] Karban J., Císařová I., Strašák T., Červenková Šťastná L., Sýkora J.: Skeletal Rearrangements Resulting from Reactions of 1,6:2,3- and 1,6:3,4-Dianhydro-beta-D-hexopyranoses with Diethylaminosulphur Trifluoride. *Org. Biomol. Chem.* 10(2), 394-403 (2012).

[5] Krupková A., Čermák Jan: Carbosilane Metallodendrimers with Cyclopentadienyldichlorotitanium(IV) End Groups. *J. Inorg. Organomet. Polym. Mater.* 22(2), 470-477 (2012).

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[8] Rychtáriková R., Šabata S., Hetflejš J., Kuncová G.: Photodynamic Efficiency of Porphyrins Encapsulated into Polysilsesquioxanes. *Chem. Pap.* 66(4), 269-277 (2012).

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[10] Slavík P., Dudič M., Flídrová K., Sýkora J., Císařová I., Böhm S., Lhoták P.: Unprecedented Meta-Substitution of Calixarenes: Direct Way to Inherently Chiral Derivatives. *Org. Lett.* 14(14), 3628-3631 (2012).

[11] Strašák T., Čermák Jan, Sýkora J., Horský J., Walterová Z., Jaroschik F., Harakat D.: Carbosilane Metallodendrimers with Titanocene Dichloride end Groups. *Organometallics* 31(19), 6779-6786 (2012).

[12] Varga V., Horáček M., Bastl Z., Merna J., Císařová I., Sýkora J., Pinkas J.: Zirconocene Silanolate Complexes and Their Heterogeneous Siliceous Analogues as Catalysts for Phenylsilane Dehydropolymerization. *Catal. Today* 179(1), 130-139 (2012).

Review papers

[13] Trögl J., Chauhan A., Ripp S., Layton A.C., Kuncová G., Sayler G.S.: Pseudomonas fluorescens HK44: Lessons Lerned from a Model Whole-Cell Bioreporter with a Broad Application History. *Sensors* 12(2), 1544-1571 (2012).

Patents

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

[15] Storch J., Církva V., Bernard M., Vokál J.: Způsob výroby [6]helicenů fotocyklizací a zařízení k jeho provádění. (Czech) Method and Apparatus for Production of [6]Helicenes. Pat. No. PV 2012-245. Applied: 12.04.11.

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
- Development of process for disposal of plastic waste using plasma pyrolysis technology
- Persistent organic pollutants and heavy metals emissions and behavior
- 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)

Applied research

- Grateless moving bed gasification of wood and waste wood
- Brownfields - Source of renewable energy (BROZEN)
- Development and verification of thermal desorption technology using microwaves
- Method for the chemical depolymerization of waste polyethylene terephthalate
- 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 biomass
- Fluidized bed combustion and gasification
- Sewage sludge combustion and co-combustion
- Optimization of waste-to-energy plant and air pollution control devices

Research projects

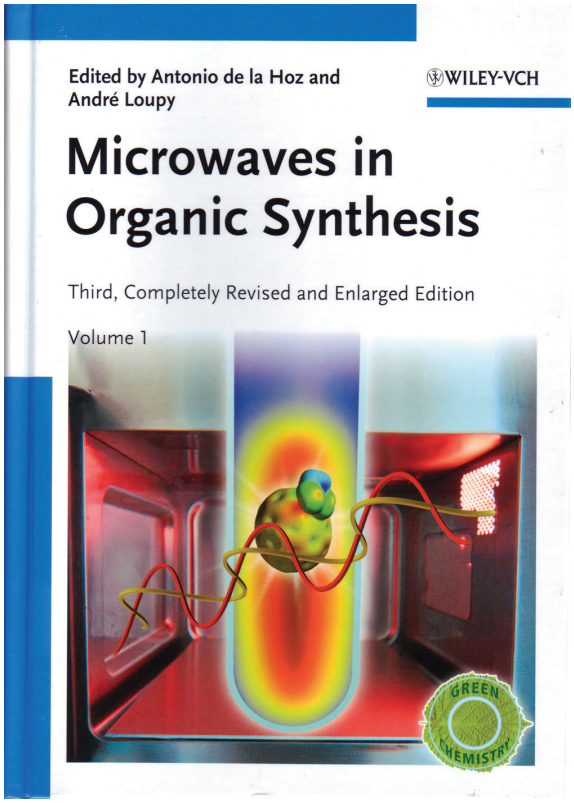
Microwaves in photochemistry and photocatalysis - overview

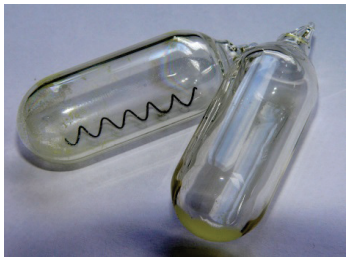
(V. Církva, cirkva@icpf.cas.cz; supported by ICPF)

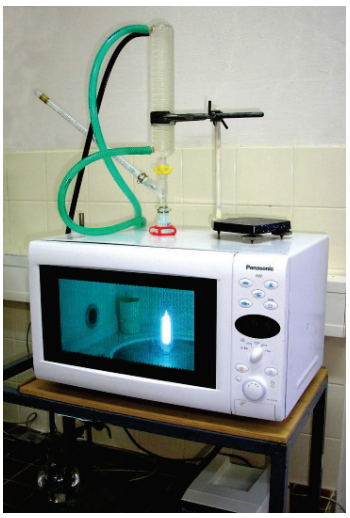
The coupled activation of photochemical and photocatalytic reactions by using of two different types of radiation, microwave and UV/Vis, is covered by the new discipline called microwave photochemistry and photocatalysis. Such a connection might have a synergic effect on reaction efficiencies or, at 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. This chapter in book is focused on the general principles of microwave photochemistry and photocatalysis, i.e. generation of UV/Vis discharge in EDLs (theory of the microwave discharges, construction of microwave-powered EDLs, preparation of the thin titania films on EDLs, spectral characteristics of the EDLs, and performance of the EDLs). Likewise, the various microwave photochemical and photocatalytic reactor types (batch with external or internal light source, flow-through with external light source, annular flow-through with internal EDL, and cylindrical flow-through surrounded with EDL) with different arrangement of the lamps have been described.

We have discussed how the concept of microwaves in photochemistry and photocatalysis is already an important issue in synthetic chemistry and material science. Although still in the beginning, detailed analysis of past and present literature confirms explicitly the usefulness of this method of chemical activation. The application of EDL simplifies the technical procedure, especially in the field of organic photochemical and photocatalytic synthesis, environmental chemistry, or analysis. [Refs. 12, 18]





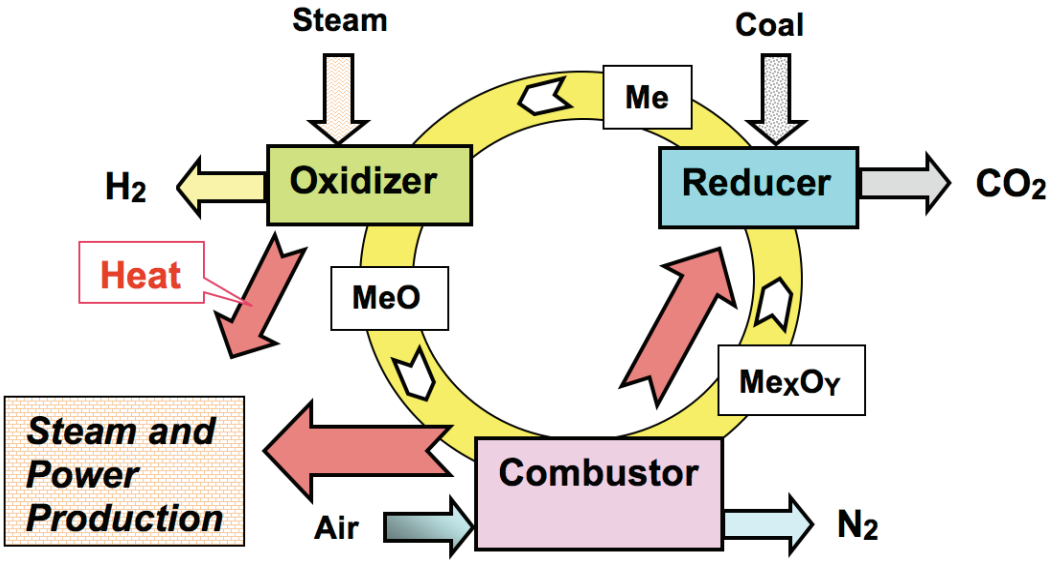


Book cover and experimental set-up for microwave photochemical reactions

Advanced processes for gasification, gas cleaning and hydrogen production - PPP bilateral Czech-Taiwanese research project

(K. Svoboda, svoboda@icpf.cas.cz; research co-operation between ICPF and Institute of Nuclear Energy Research, Longtan, Taoyuan County, Taiwan; project No. NSC 100-2911-I-042A-501)

The bilateral research project is aimed at development of advanced fluidized bed gasification processes with efficient gas cleaning and research of advanced processes for chemical looping technologies for hydrogen production. Barrier filters with fixed/moving bed of granular materials and dry medium/high temperature methods for deep removal of sulfur and chlorine compounds are studied and further developed. Also effects of staging of gasification media and effects of fluidized bed particulate materials on gasification, tar destruction and limitation of sulfur compounds emissions are among subjects of bilateral research. The target of the overall research and development is efficient combination of fluidized bed gasification with deep producer gas cleaning for long-term fuelling of solid oxide fuel cells (SOFC) and production of hydrogen and CO_2 rich streams by chemical looping processes. [Refs. 1, 2, 16]



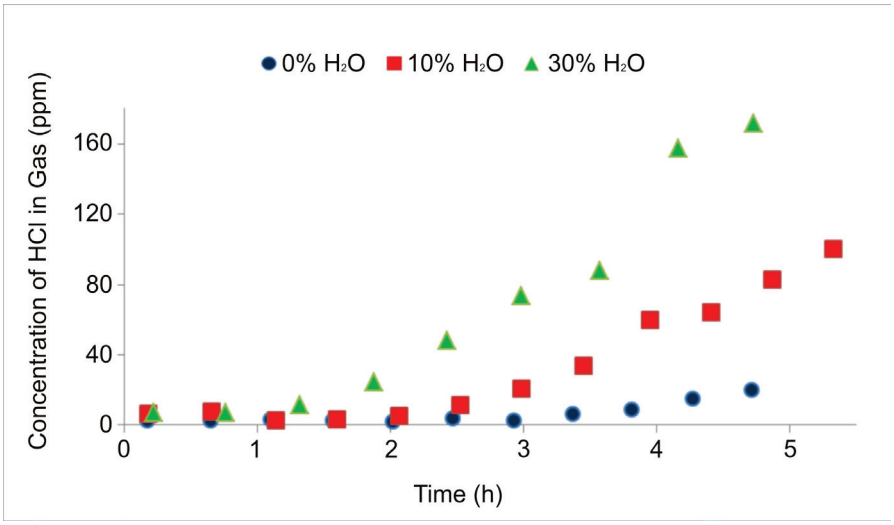
Simplified scheme of Coal Direct Chemical Looping process for hydrogen production and CO_2 separation (Me = metal, e.g. Fe)

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 (United Kingdom), ELCOGAS (Spain), UNISA (Italy); supported by MEYS and RFCS, project No. RFCR-CT-2010-00009 and 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 and 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. [Refs. 6, 8, 11, 15]



Outlet concentrations of HCl - dependence on time and water vapor concentration in gas, sorption on $KHCO_3$-alumina based sorbent (Reaction conditions: c(HCl) = 559±36 ppm-v; GHSV = 3385±215 h^{-1}), temperature = 500°C

Development of process for disposal of plastic waste using plasma pyrolysis technology and option for energy recovery

(M. Punčochář, puncochar@icpf.cas.cz; joint research project with Central Mechanical Engineering Research Institute (CMERI), Durgapur, India; supported by Joint Research Project under ASCR and Council of Scientific and Industrial Research (CSIR), India)

Plasma pyrolysis is an innovative technology for transforming high calorific plastic waste into a valuable synthesis gas (syngas) by means of thermal plasma. The process developed is a drastic non-incineration thermal process, which uses extremely high temperature in an oxygen-starved environment to completely decompose input plastic waste into syngas, composed of very simple molecules: CO, H_2 and small amount of higher hydrocarbons. A 20 kg/h capacity plasma arc pyrolyser for treatment of plastic waste as well as energy recovery options from waste plastic has been indigenously designed, developed, installed and studied its performance at the CMERI, Durgapur. After pyrolysis of plastic waste in the plasma arc reactor, generated hot gases (syngas) are quenched through water scrubbing to avoid recombination reactions of gaseous molecules; this inhibits the formation of toxic gases. Syngas composition has been characterized by Gas chromatograph; residue/ash collected at the bottom of the pyrolyser has been analyzed on Neutron Activation Analyzer (NAA). Research results indicated that the developed plasma pyrolyser might be a useful way of plastic waste treatment for energy recovery. [Ref. 7]

Experimental setup of plastic waste plasma arc pyrolyser

Moving bed gasification of biomass and biomass pellets and producer gas cleaning

(K. Svoboda, svoboda@icpf.cas.cz; contract with UJEP)

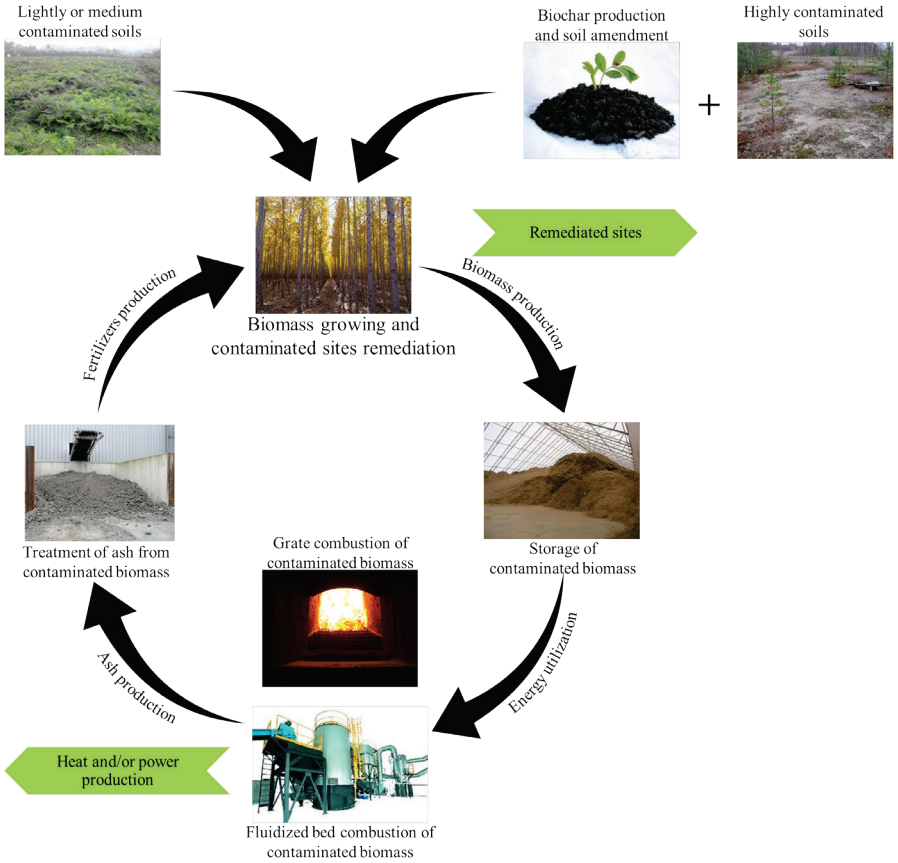
Contract dealing with experimental support for development of a new type of grateless moving bed gasifier (up-draft, co-current), production and testing of various biomass pellets for such gasification, experimental research of suitable conception for producer gas cleaning (mainly dry or wet, absorption based methods) and effects of air staging and maximum gas temperature attained on tar concentration in produced gas. [Refs. 9, 17]

Grateless moving bed gasifiers

Brownfields - Source of renewable energy (BROZEN)

(M. Šyc, syc@icpf.cas.cz; joint project with EVECO Brno s.r.o., CULS Prague; 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. [Ref. 10]



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 is 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 will be assembled. Operation efficiency of the unit will be verified by treatment of wide range of contaminated soil and solid waste

samples. By development of this innovative technology, the applicant will strengthen his market position and improve his competitiveness in the field of remediation services and hazardous waste treatment activities.

This work is focused on a pilot scale experiments of the microwave thermal desorption technology of persistent organic pollutants (POPs). Obtained results showed, that evaporization and co-transport with water vapor are main processes observed by thermal desorption. Consequently, these pollutants can be effectively removed from the solid matrix by the desorption temperature lower than boiling point of monitored contaminants. The decomposition of naturally occurring organic substances in soils was not significant during this low-temperature process (up to 240°C). On the other hand the removal efficiency for some groups of contaminants (polyaromatic hydrocarbons (PAHs) and some congeners of polychlorinated biphenyls (PCB)) was significantly lower. All contaminants were removed very effectively during temperature of batch 400°C, only efficiency of PAHs removal was just 75%. Stirring of the batch by thermal process will represent important step for rising of POPs desorption efficiency, but it could not be performed in this tests. [Refs. 5, 19]

Method for the chemical depolymerization of waste polyethylene terephthalate

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

A method for the chemical depolymerization of waste polyethylene terephthalate by application of microwave radiation and solvolysis in the presence of a catalyst comprising the first stage where the waste polyethylene terephthalate is mixed up with an microwaves absorbing activator, the mixture is melted by its exposing to a microwave radiation on a frequency from 915 to 2450 MHz and with a power output from 0.1 to 0.5 kW per kg of a charge, at a temperature from 230 to 330°C, under atmospheric pressure and the second stage, where the molten mixture is subjected to solvolysis, including acidic or basic hydrolysis, alcoholysis or glycolysis in the presence of a catalyst under continuing microwave radiation and atmospheric pressure yielding terephthalic acid, salts or esters thereof, and ethylene glycol. [Ref. 13]

Purified terephthalic acid

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 is solving the 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.

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 Prague; 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 0.3 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 1200 to 1400°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. [Ref. 14]

Afterburning furnace for incineration of the hydrogen

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

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

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

Wet separator for flying ash

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 (12 months)

Visitors

M. Čárský, University of Kwazulu-Natal, Durban, Republic of South Africa
Y. Kansha, University of Tokyo, Japan

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 Ústí nad Labem, Faculty of Environment, courses “Decontamination and Bio-remediation Technologies” and “Energetics (Power generation) and Protection of the Environment”

Publications

Original papers

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[2] Hartman M., Trnka O., Svoboda K., Pohořelý M.: Úletové rychlosti částic vápencového kalcinátu z fluidní vrstvy. (Czech) Entrainment Velocities of Calcined Limestone Particles from Fluidized Bed. *Chem. Listy* 106(4), 303-306 (2012).

[3] Kárászová M., Vejražka J., Veselý V., Friess K., Randová A., Hejtmánek V., Brabec L., Izák P.: A Water-Swollen Thin Film Composite Membrane for Effective Upgrading of Raw Biogass by Methane. *Sep. Purif. Technol.* 89, 212-216 (2012).

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[5] Mašín P., Hendrych J., Kroužek J., Kochánková L., Sobek J.: Čtvrtprovozní ověření mikrovlnné termické desorpce s reálně kontaminovanými materiály. (Czech) Verifying thermal desorption with microwave heating for real contaminated materials in a pilot scale experiments. *Acta Environmentalica Universitatis Comenianae* (Bratislava) 20(Suppl. 1), 78-83 (2012).

[6] Pohořelý M., Svoboda K., Jeremiáš M., Skoblia S., Kameníková P., Beňo Z., Šyc M., Punčochář M., Hartman M., Durda T., Krček M., Tošnarová M.: Spolu-zplyňování uhlí a dřevní biomasy ve fluidní vrstvě. (Czech) Co-Gasification of Brown Coal and Woody Biomass in the Fluidized-Bed. *Paliva* 4(4), 128-140 (2012).

[7] Punčochář M., Ruj B., Chatterj P.K.: Development of Process for Disposal of Plastic Waste Using Plasma Pyrolysis Technology and Option for Energy Recovery. *Procedia Eng.* 42(SI), 420-430 (2012).

[8] Svoboda K., Pohořelý M., Jeremiáš M., Kameníková P., Hartman M., Skoblia S., Šyc M.: Fluidized Bed Gasification of Coal-Oil and Coal-Water-Oil Slurries by Oxygen–Steam and Oxygen-CO_2 Mixtures. *Fuel Process. Technol.* 95(1), 16-26 (2012).

[9] Šulc J., Štojdl J., Richter M., Popelka J., Svoboda K., Smetana J., Vacek J., Skoblia S., Buryan P.: Biomass Waste Gasification-Can Be the Two Stage Process Suitable for Tar Reduction and Power Generation? *Waste Management* 32(4), 692-700 (2012).

[10] Šyc M., Pohořelý M., Kameníková P., Habart J., Svoboda K., Punčochář M.: Willow Trees from Heavy Metals Phytoextraction as Energy Crops. *Biomass Bioenerg.* 37, 106-113 (2012).

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[11] Pohořelý M., Jeremiáš M., Kameníková P., Skoblia S., Svoboda K., Punčochář M.: Zplyňování biomasy. (Czech) Biomass Gasification. *Chem. Listy* 106(4), 264-274 (2012).

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[13] Hájek M., Sobek J., Brustman J., Veselý V., Drahoš J.: Method for the Chemical Depolymerization of Waste Polyethylene Terephthalate. Pat. No. CN101688015/200880002443.4. Applied: 10.01.12, patented: 12.09.19.

[14] Lederer J., Kovač D., Veselý V., Hanika J., Nečesaný F.: Způsob výroby vodíku parciální oxidací vysokovroucích uhlovodíkových směsí a biomasy, a zařízení k provádění způsobu. (Czech) Process for Hydrogen Production by Partial Oxidation of High Boiling Hydrocarbon Mixtures and Biomass, and Apparatus for Processing. Pat. No. CZ303392/PV 2010-653. Applied: 10.09.02, patented: 12.08.29.

[15] 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. CZ24582/PUV 2012-26461. Applied: 12.07.27, patented: 12.11.19.

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[19] Hájek M., Sobek J., Mašín P., Hendrych J., Kroužek J., Kubal M., Kukačka J.: Způsob dekontaminace tuhých materiálů. (Czech) Method of Decontamination of Solid Wastes. Pat. No. PV 2012-269. Applied: 12.04.19.

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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
- IR and UV laser photopolymerization in the gas phase
- UV laser chemical liquid deposition of metal nanosols and nanocomposites
- CVD of nanostructured objects (nanowires, nanoplatelets)
- IR and UV laser deposition of TiO_2-based materials
- IR and UV laser ablation for deposition of thin films

Research projects

Aerosols, Clouds, and Trace gases Research InfraStructure Network

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

ACTRIS (Aerosols, Clouds, and Trace gases Research InfraStructure 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".

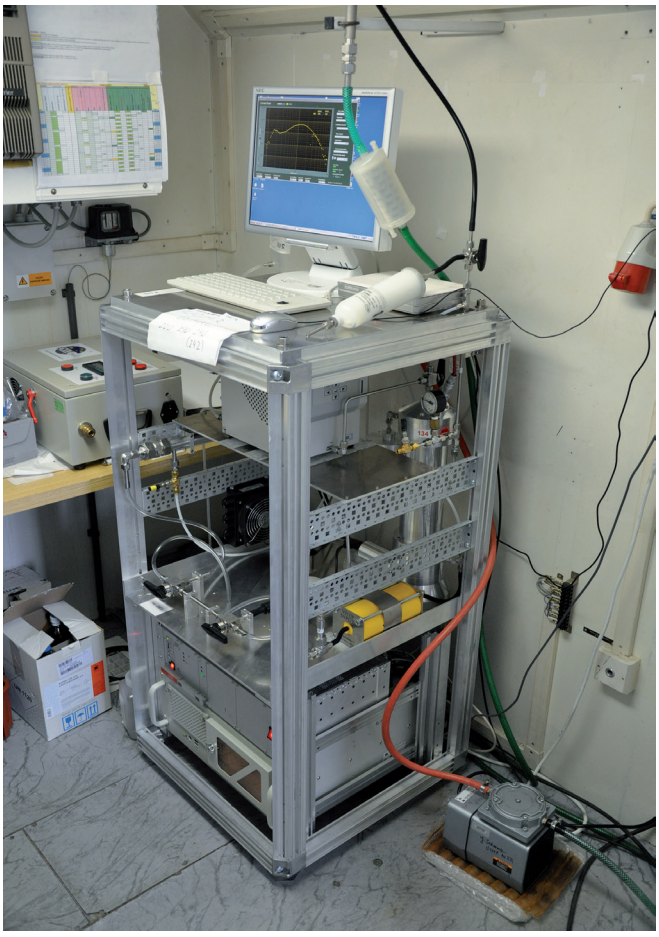


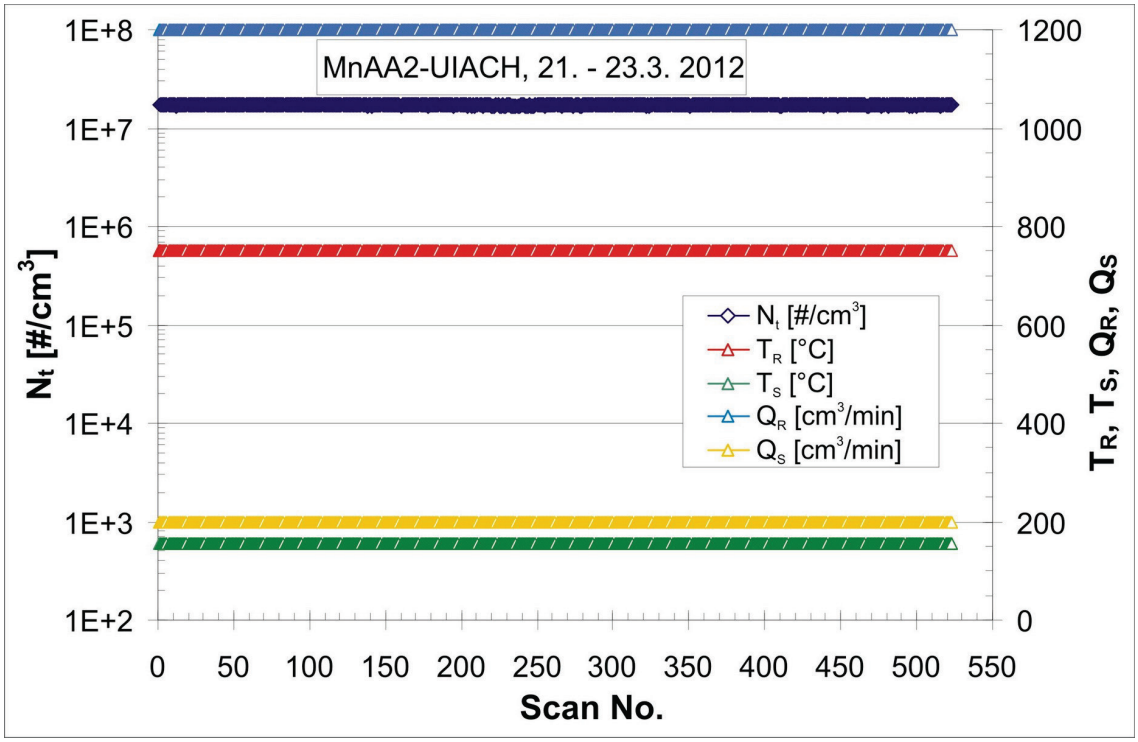
Photo of the scanning mobility particle sizer measuring size distribution of particles at background site Košetice

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.



Time dependence of number concentration N_t of MnO_x nanoparticles generated in purified nitrogen at given T_R, T_S, Q_R, Q_S. 1 scan = 5 minutes. Notice a stable output concentration during 45 hours of the experiment

Thermophysical properties of water in unexplored, technologically significant regions

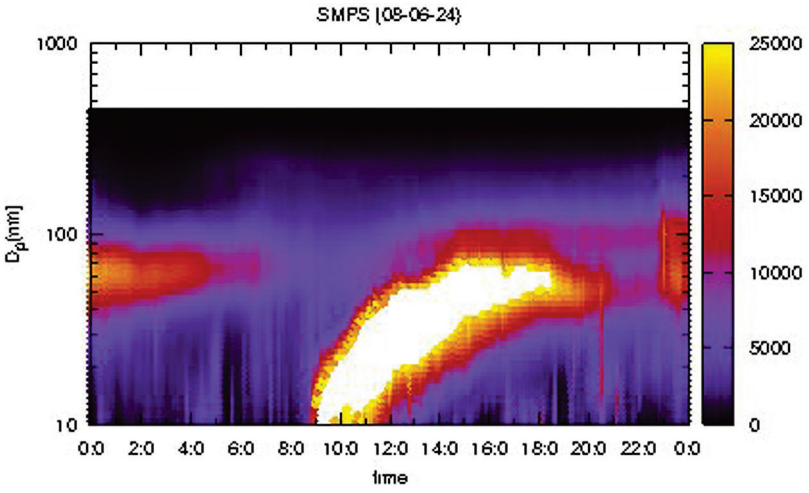
(V. Ždímal, zdimal@icpf.cas.cz; joint project with Institute of Thermomechanics of the ASCR, v. v. i., CTU, and University of West Bohemia, Plzeň, supported by GA ASCR, project No. IAA4200760905)

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. 7, 8]

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. 2, 10, 13]

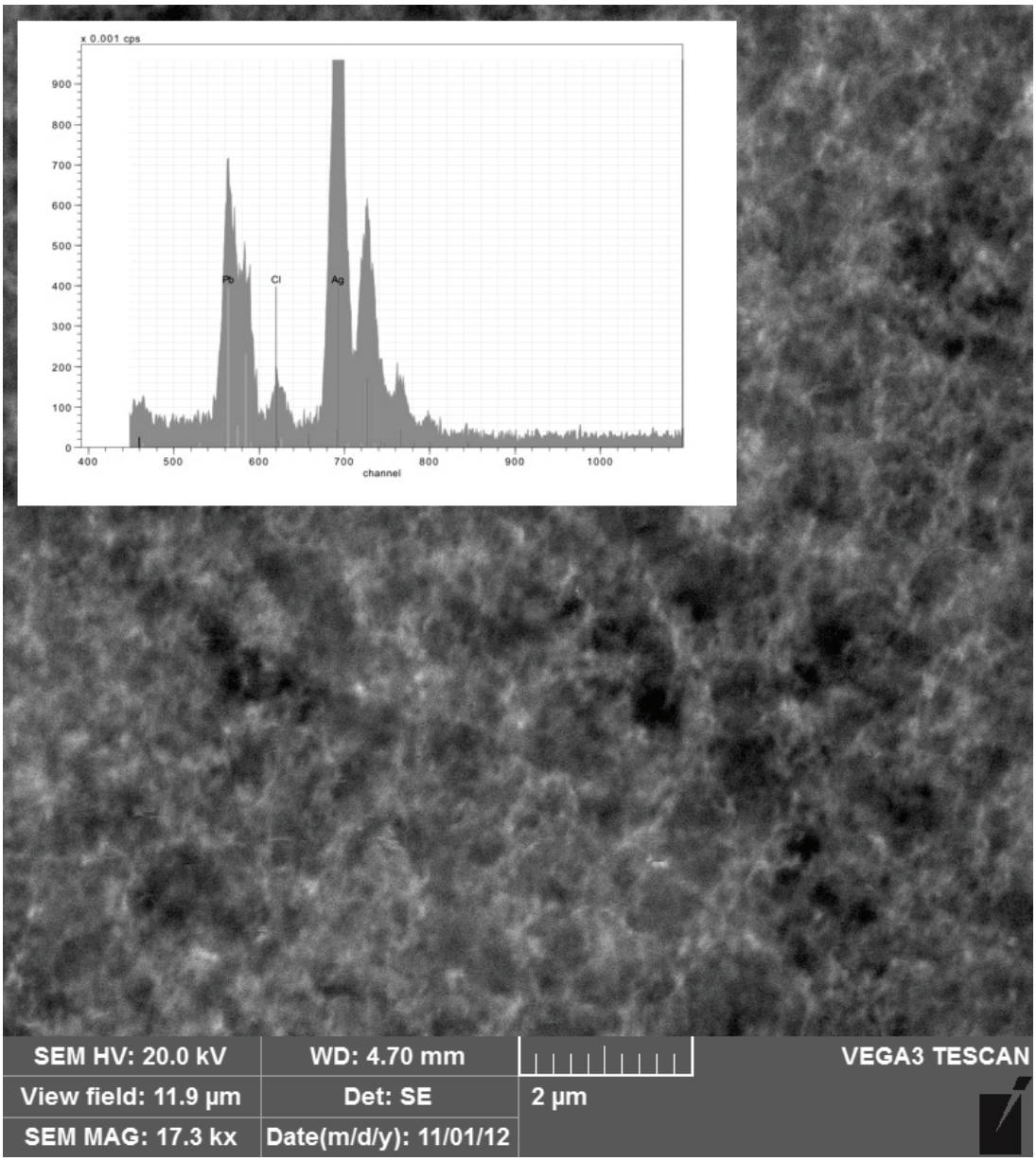


New particle formation event "banana type"recorded by aerosol spectrometer SMPS at rural background station Košetice

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.



Pb nanoparticles and their EDS spectrum (inset) generated by PVD method for inhalation experiments

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, v.v.i.; 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. [Refs. 7, 8]

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.

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.

Preparation of thin layers of ferromagnetic semiconductors

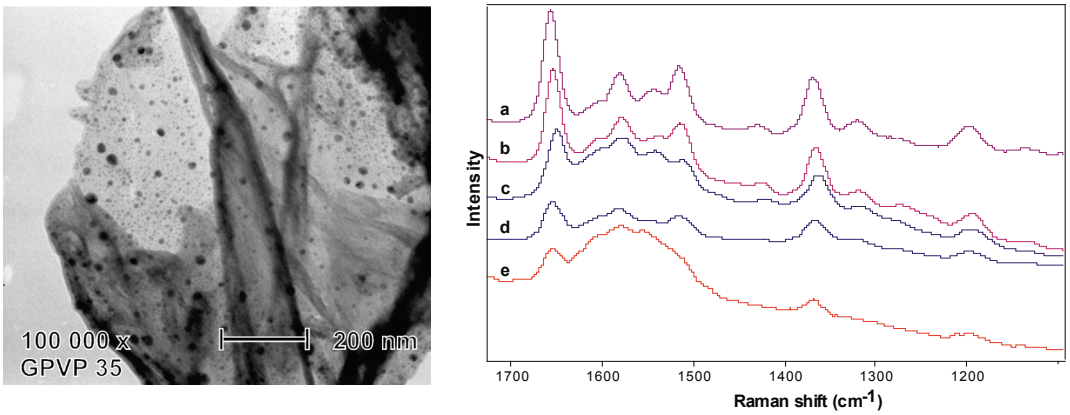
(R. Fajgar, fajgar@icpf.cas.cz; supported by ICPF)

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.

Novel sensors based on laser ablated graphene

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

Nanocomposites of poly(BA/MMA) reinforced with up to 3 wt. % graphene sheets were used as targets for laser ablation. The target was ablated using TEA CO_2 laser with fluence of 1.00 J/cm^2 and thin films of crosslinked polymer with embedded graphene sheets with large specific surface area were obtained. The polymer-graphene deposit was covered with silver nanoparticles by excimer laser ablation in order to prepare active substrates for Surface-Enhanced Raman Scattering (SERS). In vacuum, Ag nanoparticles reaching the polymer/graphene substrate graphitized the graphene as revealed by Raman spectroscopy. Optimized ablation in helium atmosphere was used to preserve graphene covered with silver nanoparticles. The nanocomposites were characterized by means of spectroscopies, microscopies and diffraction technique. 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.



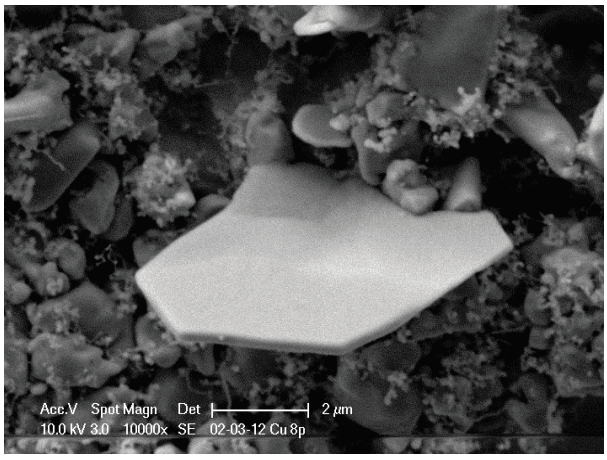
(a) (b)

(a) SEM image of the SERS active substrate (Ag nanoparticles on the graphene surface)
(b) Raman spectra of Rhodamine 6G on Ag/graphene support (lines a-10^{-4}, b-10^{-5}, c-10^{-6}, d-10^{-7} mol/l) and Ag alone (line e -10^{-5} mol/l)

Formation of Cu_xGe_y nanoplatelets using LPCVD of hexamethyldigermane (Ge_2Me_6) and tetraethyllead ($PbEt_4$)

(V. Dřínek, drinek@icpf.cas.cz; supported by ICPF)

Low Pressure Chemical Vapor Deposition (LPCVD) of Ge_2Me_6 and $PbEt_4$ allows decomposition of both gaseous compounds and leads to deposition of nanoplatelets along with Ge nanowires, and nanoparticles. In agreement with analytical techniques (Raman spectroscopy, ED, EDX, SEM and HRTEM) the nanoplatelets up to several tens of mm in length have been prepared in solid solution of Ge in Cu cubic lattice. Thickness of the nanoplatelets ranges from 100-400 nm. Nanowires which are composed of cubic Ge have a diameter of about 30 nm and length of several tens of micrometers. Lead was detected in amorphous phase of around dispersed nanoparticles. [Ref. 5]



Ge/Cu platelet prepared by CVD process

IR laser photochemical deposition of amorphous Fe/Si nanocomposite films and thermal evolution of nanocrystalline grains of ferrisilicate, carbon-encapsulated iron disilicide and rare high-pressure ambient conditions-surviving hexagonal iron

(J. Pola, pola@icpf.cas.cz; no support)

IR laser-induced gas-phase co-photolysis of $Fe(CO)_5$-SiH_4 mixtures occurs as SiH_4-photosensitized $Fe(CO)_5$ decomposition enhanced by products of $Fe(CO)_5$ decomposition and

it results in deposition of amorphous Si/Fe nanocomposite films. The analyses of the deposited and subsequently annealed solid films were made by FTIR, Raman and X-ray photoelectron spectroscopy, X-ray diffraction and electron microscopy. The deposited films are amorphous, undergo atmospheric oxidation in topmost layers to iron oxide and hydrogenated silicon oxide and contain crystalline nanostructures of iron silicide $FeSi_2$. Upon annealing they develop nanocrystalline structures of ferrisilicate $Fe_{1.6}SiO_4$, carbon-encaged iron disilicide $FeSi_2$ and very rare hexagonal (high-pressure) Fe surviving ambient conditions. Mechanism of formation of these nanostructures is discussed in terms of gas-phase and solid-phase reactions. [Refs. 11, 12, 14]

Quantum size effect in semiconductor nanostructures for optoelectronics

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

Thin layers of non-hydrogenated and 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.

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 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 Eastern Finland, Kuopio, Finland: Novel aerosol generation processes focused on medical treatment and nanotechnology

University of Vienna, Faculty of Physics, Dept. of Aerosol physics and Environmental Physics, Vienna, Austria: Black and elemental carbon analysis, aerosol optical properties

Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodź, Poland: UV laser-induced cross-linking of polysiloxanes

Faculty of Technology and Metallurgy, University of St. Cyril & Methodius, Skopje, Republic of Macedonia: Novel preparation and photocatalytic study of titania-based catalysts

Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of nanosized metal chalcogenides and polycarbosilathianes

King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia: Laser degradation of contaminants in fuel oils
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
University of Crete, Heraklion, Greece: Laser induced chemical vapor deposition of polycarbosilathianes
AC2T, Wiener Neustadt, Austria: Tribological study of nanostructured materials (nanowires, nanoplatelets)

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
J. Blazevska-Gilev, University of St. Cyril & Methodius, Skopje, R. Macedonia
Radmila Tomovska, POLYMAT, Institute for Polymer Materials, San Sebastian, Spain
Nicole Doerr, AC2T, Wiener Neustadt, Austria
Josef Brenner, AC2T, Wiener Neustadt, Austria
Ulrike Cihak – Bayr, AC2T, Wiener Neustadt, Austria

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] Blazevska-Gilev J., Urbanová M., Pokorná D., Šubrt J., Pola J.: IR Laser-Induced Breakdown in Thiirane for Gas-Phase Deposition of Conjugated Organosulfur Polymer Incorporating Cycloheptasulfur. *J. Anal. Appl. Pyrol.* 93, 165-169 (2012).

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Patents

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K. AIM: International Steering Committee, 26th European Symposium on Applied Thermodynamics (ESAT 2012), Potsdam, Germany, 7-10 October 2012 (http://events.dechema.de/events/en/Events/Events+Archive/ESAT+2012/Committee-p-126302.html)
K. AIM: 2nd Vice-Chair (formerly Delegate to the High Level User Group), Board of Governors, Joint Research Centre, European Commission (http://ec.europa.eu/dgs/jrc/index.cfm?id=1480)
K. AIM: Co-Chair, Member of Organization Forum on Science Foresight for Joint Strategy Development, European Science Foundation (http://www.esf.org/coordinating-research/mo-fora/science-foresight-for-joint-strategy-development.html)
K. AIM: Working Party on Thermodynamic and Transport Properties, EFCE (http://www.efce.info/wp.html)
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J. DRAHOŠ, I. WICHTERLE, P. KLUSOŇ: Board of the Congress, 20th International Congress of Chemical and Process Engineering CHISA 2012, Prague, 25–29 August, 2012 (http://www.chisa.cz/2012)
P. IZÁK: Member of „European Membrane Society Board”
P. IZÁK: Scientific Committee, Euromembrane 2012, Imperial College London, UK, 23-27 September, 2012 (http://www.euromembrane2012.com/conference-committee.html)
J. SMOLÍK: President of the European Aerosol Assembly (EAA) Board (2010-12) (http://www.gaef.de/eaa/)
J. SMOLÍK: Member of “Committee on Nucleation and Atmospheric Aerosols” (http://www.icnaa.org/committee.html)

14TH E. HÁLA LECTURE (2012)

JAROSLAV ŠESTÁK (New Technologies Research Centre, University of West Bohemia)
"Energetika dnes a zítra: politika versus zdravý rozum vědy a techniky" (Czech)
"Power engineering today and tomorrow: politics versus common sense of science and technology"

ACRONYMS USED THROUGHOUT THE REPORT

ASCR	Academy of Sciences of the Czech Republic
BAS	Bulgarian Academy of Sciences
CNRS	Centre Nationale de la Recherche Scientifique
CTU	Czech Technical University in Prague
CU	Charles University in Prague
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
IMC	Institute of Macromolecular Chemistry of the ASCR, v. v. i., Prague
JH IPC	J. Heyrovský Institute of Physical Chemistry of the ASCR, v. v. i., Prague
KIT	Karlsruhe Institute of Technology
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
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
TACR	Technology Agency of the Czech Republic
TU	Technical University
UJEP	Jan Evangelista Purkyně University in Ústí nad Labem, Czech Republic
VOCs	Volatile Organic Compounds

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Vladimír Církva (Editor)

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