INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS

OF THE ASCR, V. V. I.

ANNUAL REPORT 2010

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On 18 May 2010, Institute of Chemical Process Fundamentals of the ASCR celebrated the 50th Anniversary of its establishment. A bronze bust of the Institute's founder Prof. Vladimír Bažant was unveiled in vestibule on this occasion.

(The bust was crafted by Prof. Zdeněk Herman)

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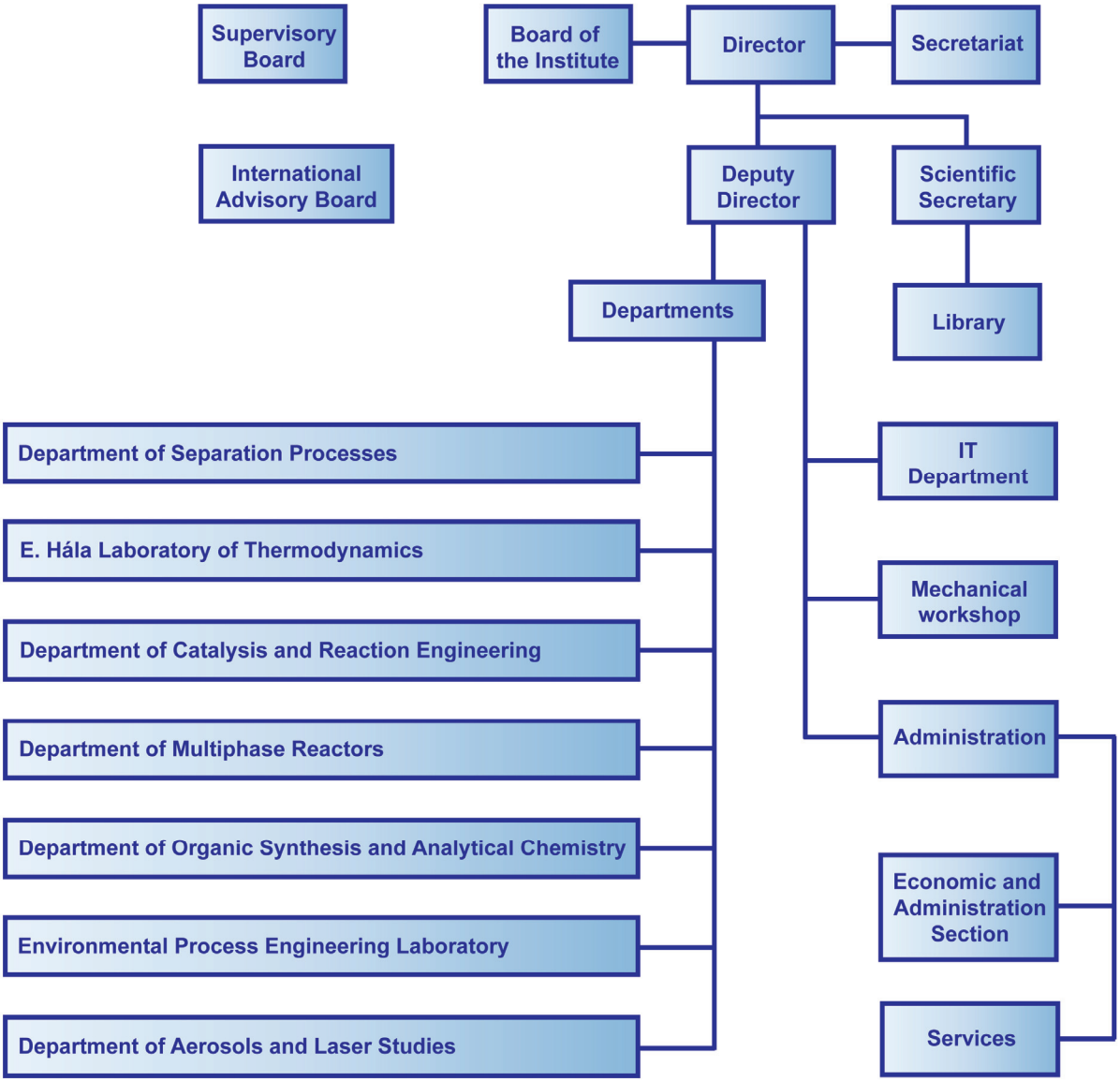
Organization Chart



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 PhD studies in the field of chemical, biochemical, environmental engineering and processes, physical chemistry, organic chemistry, industrial chemistry, and biotechnology.

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STAFF

(December 31, 2010)

Category	Number of Employees
Research	143
Technical	14
Administrative	15
Services	12

BUDGET 2010

(18 CZK ≈ 1 US$, 25 CZK ≈ 1 €)

Resources	Million CZK
Institutional support based on Institutional Research Plan	120
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	57
Foreign R&D Funds and European Programmes	6
Contracts with industry	4
Total Resources	187

Expenses	Million CZK
Personal expenses including mandatory insurance	91
Purchase of material	19
Purchase of services	11
Repairs and maintenance	20
Depreciation of fixed assets	30
Travel expenses	6
Energy, water, and fuels	6
Total other expenses	4

Department of Separation Processes

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TECHNICAL STAFF
DAVID KARFÍK, MARTA KOPTOVÁ, DALIBOR VLČEK
Part time: ALENA KADLECOVÁ, JÚLIUS MAŠČENÍK

Fields of research

- Research and development of electrochemical bipolar microreactor for alkoxylation
- Hydrodynamics of two phase flow in narrow channel
- Sulfur dioxide oxidation, sulfation and sulfonation
- Integrated multiscale process units with locally structured elements
- Liquid-liquid extraction of tall oil from wastewaters of paper industry
- Fluorinated hydrocarbons as potential solvents in liquid-liquid extraction processes
- Supercritical fluid extraction of biologically active substances
- 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 vapours from air by supported ionic liquids membranes

Applied research

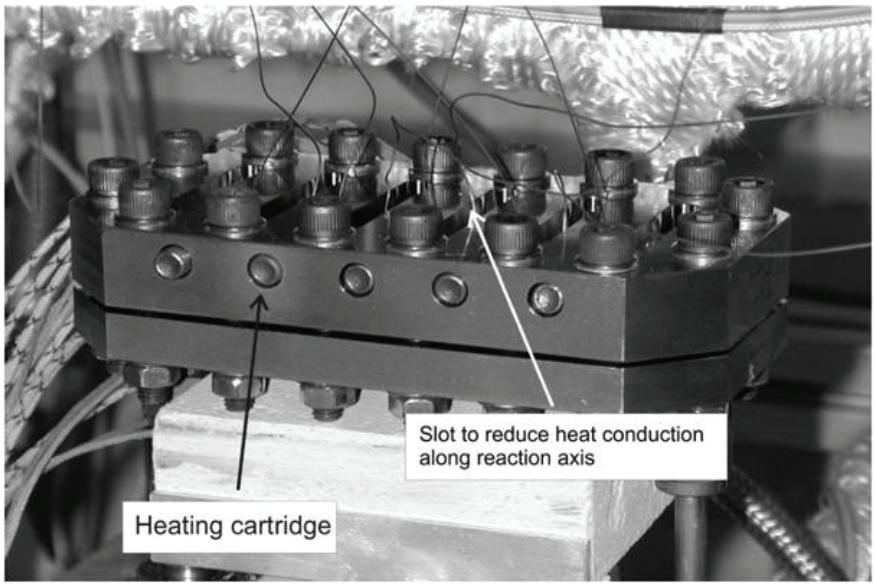
- Research and development of new methods of emulsification using microtechnology
- Hydrodynamic characterization of micromixers
- Extraction and production of plastic modifiers for production of tyres
- Liquid extraction of luminophores, recycling of Y and Eu
- Liquid and supercritical fluid extraction and refining of plant extracts
- Purification of biogas by supported ionic liquid membrane
- Reclaiming of phytosterols and other valuable compounds from tall soap/oil

Research projects

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

(V. Jiřičný, 7th FP 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. Project is deliver new production mode based on plug-and-play modular production technology and holistic process design methodology applying intensification concepts and innovative decision tools. ICPF in cooperation with Procter&Gamble (leader of subtask) and KIT Karlsruhe are involved in research and developments of sulfur dioxide oxidation, sulfation and sulfonation. The mathematical model for sulfur dioxide oxidation has been developed in ICPF. Model was validated with experimental data conducted on microreactor developed and manufactured by KIT Karlsruhe. Simulations with the model were used for development and design of new microreactor. [Refs. 1, 25, 37, 62, 63, 70].

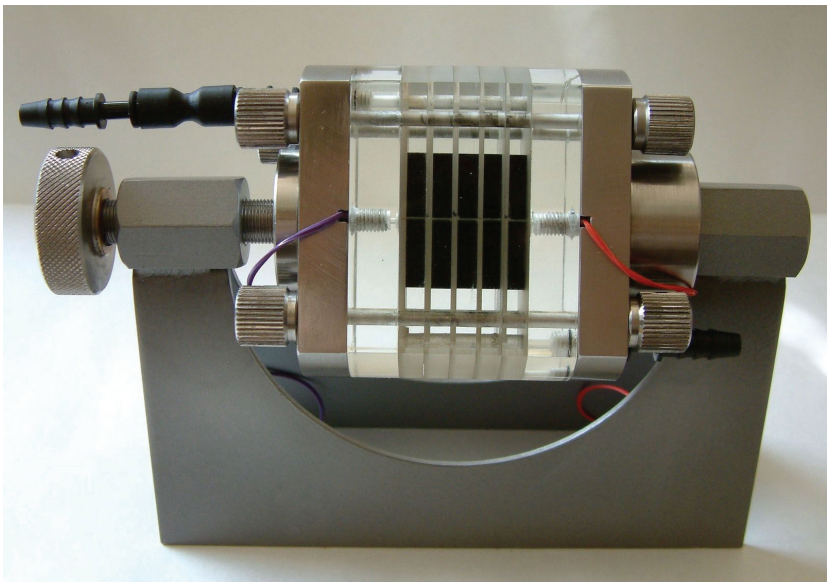


Photograph of the lab scale reactor for SO_2 oxidation with slotted holes in the cover plate and holes for the heat cartridges designed and manufactured in KIT

Chemical degradation of polybrominated diphenyl ethers

(V. Jiřičný, supported by GACR, project No. GA104/09/0880)

Polybrominated diphenyl ethers (PBDEs) are widely used as flame retardants, mainly for polymers and textiles. PBDEs have an ideal property for these matrices because they are decomposed at temperature 50 °C lower than point of flammability of matrix. PBDEs are pollutants of environment. They are lipophilic, potential carcinogenic and neurotoxic compounds, which accumulate in environment and they can migrate by food chain into human organisms. The various methods of degradation of PBDEs have been experimentally verified. The best and original results have been conducted with electrochemical micro-reactor. The reliable GC analytical method has been developed. [Refs. 26, 43, 46, 67-69].



Filter-press type bipolar electrochemical microreactor designed and manufactured in ICPF

Research and developments of new methods of emulsification using microtechnology

(J. Křišťál, contract with Procter&Gamble, ICPF Contract No. 171020)

The contract is focused on the development of new methods for production of very stable emulsions. Microtechnology equipments are used in this research to reach the desired goals. Results are published in confidential Procter&Gamble research reports.

Research and developments of various microapparatus characteristics

(J. Křišťál, contract with Procter&Gamble, ICPF Contract No. 171050)

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

Integrated multiscale process units with locally structured elements

(J. Hanika, IMPULSE, 6FP integrated project)

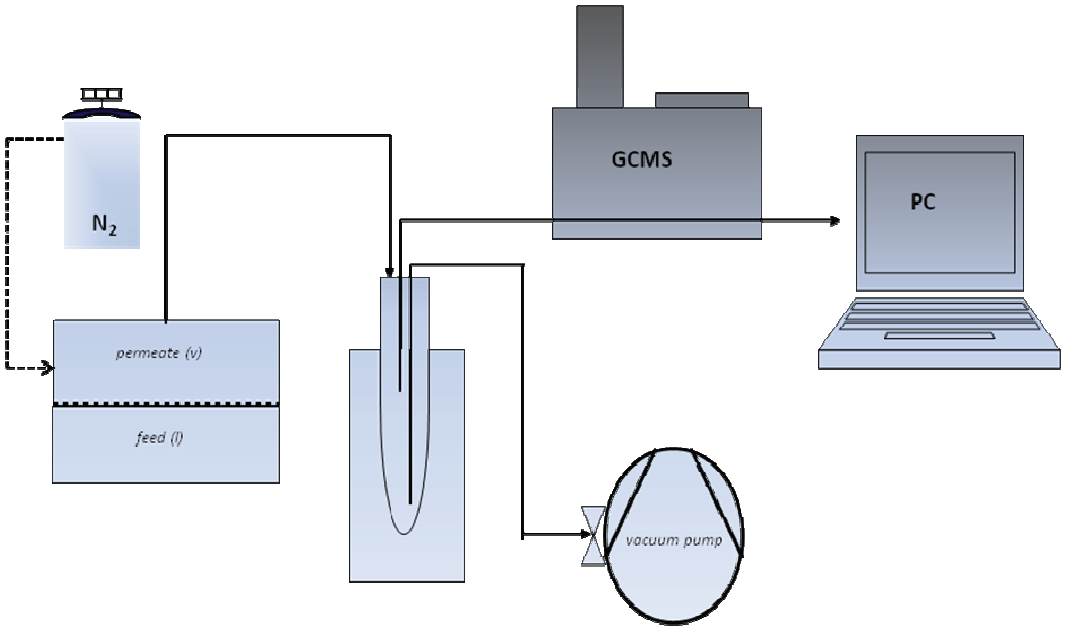
The objective of project is effective, targeted integration of innovative process equipment such as microreactors, heat exchangers, thin-film devices and other micro components to attain radical performance enhancement for whole process systems in chemical production. We are involved in the application research of electroorganic synthesis in electrochemical micro-reactor. Bipolar electrochemical microreactors proved advantages of microtechnology. While conversion and selectivity of the process are comparable with conventional process, the main profit of applied microtechnology is in less expensive separation of the product from reaction mixture. [Refs. 3-5, 27, 38-40, 64-65]

Ionic membranes for selective separation of liquid mixtures by pervaporation

(P. Izák, joint project with ICT, supported by GACR, grant No. GA104/08/0600)

In this project, we evaluated the effect of ionic liquid to the equilibrium solvent (butan-1-ol) vapour sorption in PDMS and effects of the ionic liquid content on the sorption and desorption kinetics of butan-1-ol, all at 37 °C. The generalized Fick's second law, solved at

time dependent boundary conditions occurring in the apparatus, provided a satisfactory approximation of the data on sorption and desorption kinetics of butan-1-ol vapour in PDMS and in the PDMS–ionic liquid blends; the resulting values of diffusion coefficient depended on the choice of the equilibrium vapour sorption model. The significant decrease of diffusion butan-1-ol diffusion coefficients at equilibrium activities above approx. 0.6 indicate anomalous sorption and desorption of butan-1-ol at higher concentrations in the membranes investigated. The increased content of the benzyl-3-butylimidazolium tetrafluoroborate ionic liquid in the PDMS based membranes positively influenced the equilibrium concentration of butan-1-ol in such membranes over the whole butan-1-ol vapour activity interval and, at the same time, reduced the butan-1-ol diffusion coefficients. [Refs. 7, 12-14, 18, 28, 30, 41, 42, 44, 49].

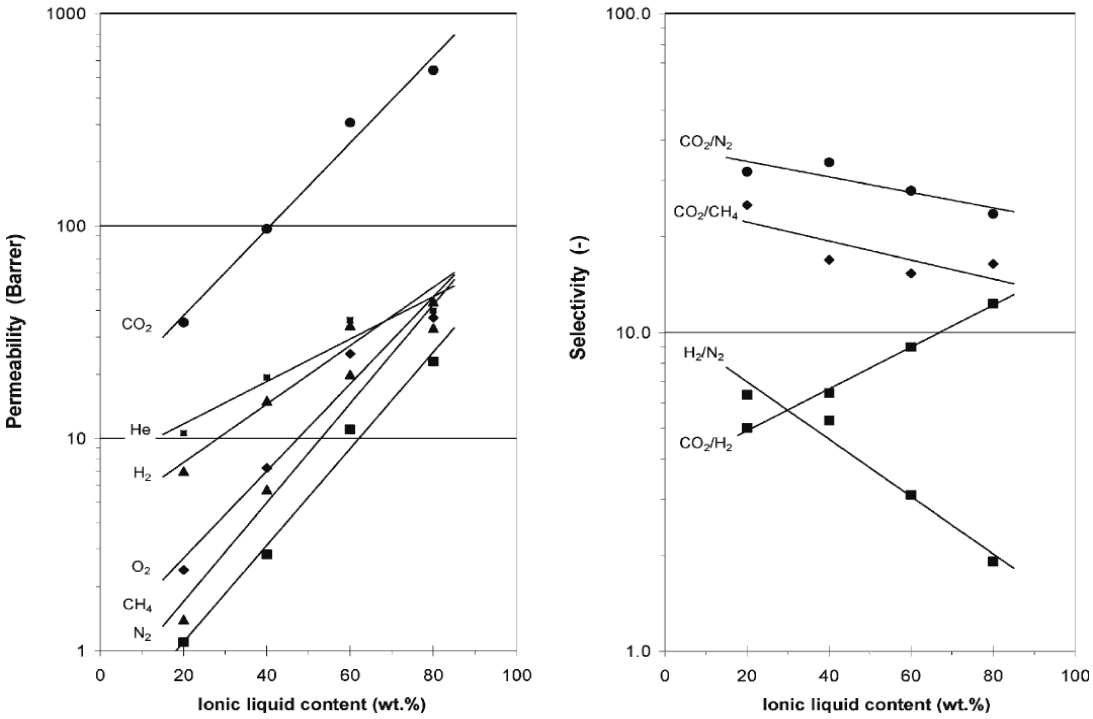


Scheme of pervaporation apparatus

Separation of volatile organic compounds from air

(P. Izák, joint project with ICT, supported by GACR, grant No. P106/10/1194)

Outflow of vapours of volatile organic compounds (VOCs) leaking from gasoline during its storage, transportation and handling is a serious ecological problem due to the toxicity of these compounds (e.g. some of them can cause a cancer). It is also an economical problem connected with the loss of a valuable industrial product. Although amounts of gasoline vapours lost during common operations like handling and storage may seem negligible, they reach hundreds of tons per year. All above mentioned facts are the reason, why the separation of these compounds from air and their recycling is critically important. The aim of this project is finding of a convenient separation method of VOCs from the air based on new approach to the problem (using of room temperature ionic liquid (RTIL) or modified polymer membrane). [Refs. 6, 29].

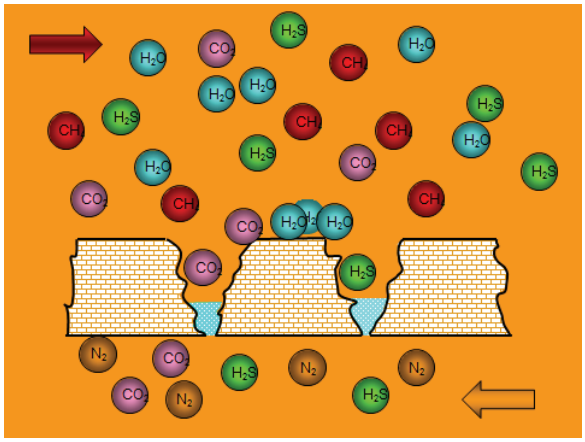


Permeability of six permanent gases as a function of the IL content (left) and corresponding selectivity between selected gas pairs (right)

Purification of biogas by supported ionic liquid membrane

(P. Izák, joint project with Česká hlava s.r.o., supported by MIT, project No. ER-TI1/245)

A new method for raw biogas purification from impurities and carbon dioxide separation by "condensing liquid membrane" was verified. The hydrophilic porous membrane helped to form under condensing condition (below dew point of the raw biogas feed) a very thin selective water layer. Major difference in permeability of certain raw biogas components (carbon dioxide, hydrogen sulfide) and methane through water layer is responsible for high upgrading of raw biogas to biomethane quality. Condensing liquid membrane is also environmentally friendly because it produces no toxic waste and the separation may become a part of waste water treatment. It represents a new approach to production of biofuel from biogas. [Refs. 6, 11, 19, 33, 34, 47, 48].

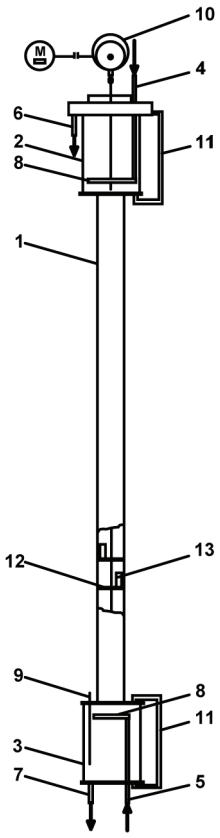


Impurities and CO_2 in raw biogas are separated by a "condensing-liquid membrane", based on the different solubility of components in a very thin layer in a porous membrane

Reclaiming of phytosterols and other valuable compounds from tall soap/oil

(M. Rousková, A. Heyberger, joint project with Technological Park in Chomutov and Institute of Systems Biology and Ecology ASCR)

The aim of the project is to study the tall soap composition and to develop methods of extractive separation of the valuable compounds. Besides of working out the necessary analytical methods, the extraction equilibria in systems with various solvents were measured, and the separation processes were simulated in a laboratory vibrating plate extraction column. A novel extraction processes and equipment have been designed for recovering phytosterols and unsaturated fatty acids from tall soap. [Refs. 15, 21-23, 31, 32, 50, 54]



Symbols used

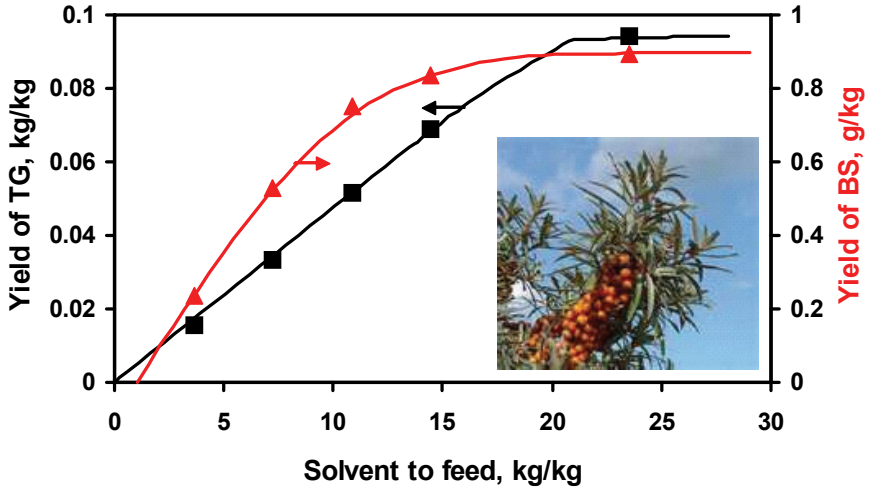
1 column coat
2 upper settler
3 lower settler
4 inlet of heavier phase (soln. of tall soap)
5 inlet of lighter phase (solvent)
6 outlet of extract
7 outlet of raffinate
8 liquid distributor
9 control of interphase boundary
10 eccentric drive
11 liquid level control
12 perforated plates
13 downcomers for continuous phase

Scheme of the vibrating plate extractor (VPE)

Supramolecular materials based on natural phytosterols for applications in biology

(H. Sovová, joint project with IOCB, ICT, and Chemispol s.r.o., supported by MEYS, project No. 2B06024)

Supercritical fluid extraction of β-sitosterol as a component of sea buckthorn and sunflower oils was studied in detail. The experimental data on the effect of extraction conditions on the yield and extract composition were interpreted in relation to phase equilibrium. This approach was verified on literature data on the extraction of carotenoids with oil. A sitosterol-enriched fraction was obtained using two separators. An alternative resource of β-sitosterol was stinging nettle root. The potential of enzymatic reactions of vegetable oils in supercritical carbon dioxide to enhance the concentration of minor components was studied. 20-hydroxyecdysone enrichment up to 12 wt. % in a fraction of *Leuzea carthamoides* CO_2 extract was achieved using ethanol as entrainer [Refs. 16, 17, 52, 53, 55, 56, 61].

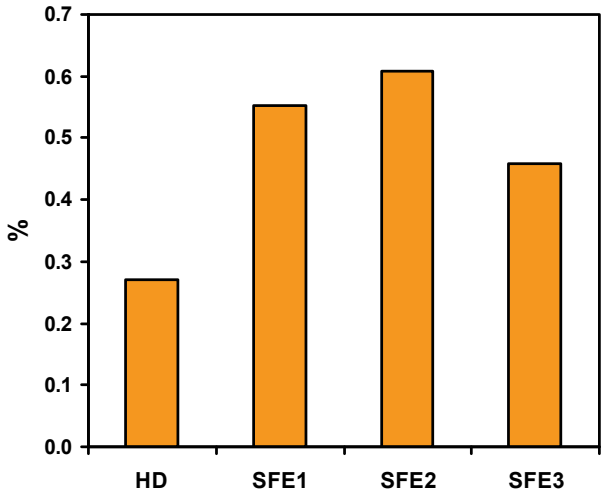


Extraction of oil from sea buckthorn seeds with CO_2 at 60 °C and 28 MPa: β-sitosterol is extracted faster than triglycerides, the major component

Optimization of supercritical fluid extraction for maximal yield of biologically active substances from plants

(H. Sovová, joint project with Research Institute of Plant Production and Agra Group, supported by MEYS, project No. 2B06049)

The kinetics of supercritical fluid extraction of different essential oils was described with a phenomenological model. Strong insecticidal activities of *Tanacetum parthenium* extracts were observed and quantified in dependence on extraction conditions. Applications for a patent on *Ruta graveolens* based means for plant protection against pests were submitted. The operational conditions of savory extraction with respect to thymoquinone and other volatile oil components in the extract were optimized. The composition and insecticidal activity of extracts from four *Lamiaceae* plants were compared with the aim to find the active extract components [Refs. 2, 9, 35, 36, 51, 56, 57].

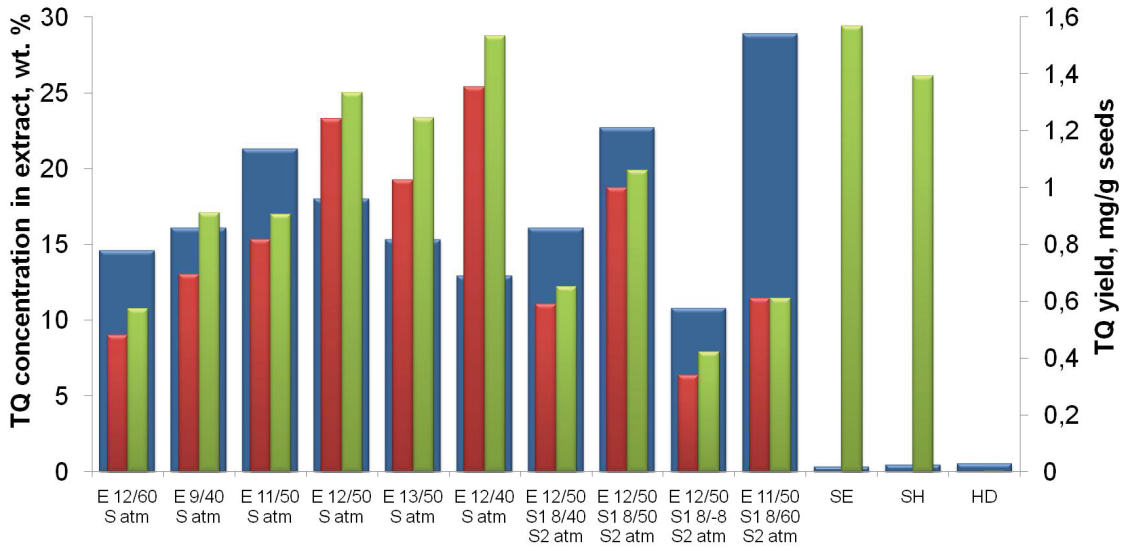


The yield of identified essential oil components (%, w/w) isolated from *Tanacetum parthenium* by hydrodistillation (HD) and supercritical CO_2 extraction (SFE1-3)

Determination of biological activity and chemical composition of selected tropical and subtropical Ranunculaceae species

(H. Sovová, joint project with Czech University of Life Sciences, and IOCB, supported by GACR, grant No. GA525/08/1179)

The research was focused on the enhancement of thymoquinone (TQ) concentration in CO_2 extracts of black cumin (*Nigella sativa* L.) seeds using two separators. With respect the TQ yield and its concentration in extract, the best results were obtained at 12 MPa and 50 °C in the extractor and 8 MPa and 50 °C in the first separator. The yield was 1.0 mg TQ/g seeds and 22.7 wt. % TQ in the extract [Ref. 58].



Supercritical fluid extraction of thymoquinone from *Nigella sativa* seeds (E) is more efficient and selective than Soxhlet extraction with ethanol (SE) or hexane (SH) and than hydrodistillation (HD): blue: TQ concentration in 1st fr. of extract, red: yield of TQ in 1st fr., green: total yield of TQ

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

(P. Uchytil, joint project with IMC, supported by the GACR, Grant No. GA104/09/1165)

The relation between polymeric structure of pervaporation membranes on the basis of poly-γ-benzyl-L-glutamate and their transport properties was studied with the group of Dr. S. Kononova (IMC). The pervaporation of binary mixture toluene and heptane was measured. High separation was achieved. Paper with the results was accepted in Crystallography Reports [Ref. 8, 45].

Preparation of dense homogeneous polymeric membranes and study on their gas permeation properties

(P. Uchytil, joint project with National Chung Hsing University, Taiwan, supported by ASCR and by National Science Council of Taiwan, project No. P106/10/J038)

The project is focused on the study of carbon dioxide and methane transport in a poly(vinylidene fluoride-co-hexafluoropropylene) polymeric membrane (Viton) containing ionic liquid. Two ionic liquids 1-hexyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide ([HMIM][TFSI]) and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][TFSI]) were used for preparation of ionic liquid membranes. The transport properties of these membranes were tested using dynamic permeation method [Ref. 66].

Mass transport during membrane permeation and pervaporation

(P. Uchytil, joint project with University of Colorado, Boulder, USA, supported by MEYS, KONTAKT project No. ME 889)

A new apparatus for gas permeability, diffusivity and solubility assessing in dense polymeric membranes was constructed and his function was verified. Toluene transport model based on data from the new permeation apparatus was proposed. The theoretical and experimental study of butane and isobutane vapour flow through porous Vycor glass membrane with pore size between 20 and 200 nm under different conditions was performed. The experiment results and predicted results were compared with an adiabatic model [Refs. 20, 10, 24, 59, 60].

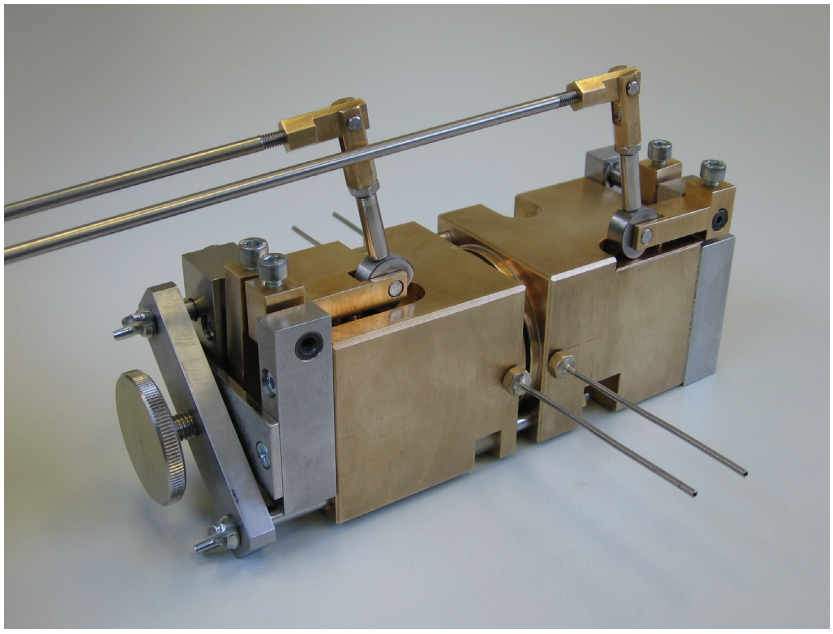


Photo of a new type of the permeation cell for determination of transport parameters in polymeric membranes

International co-operations

CNRS Toulouse, France: Characterization of two phase flow in microchannels
CNRS Lyon: Hydrogenation in falling film microreactor
CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials
Institute of Chemical Engineering, Sofia, Bulgarian AS: High-pressure phase equilibria
Institute of Macromolecules, St. Petersburg, Russian Academy of Science, Russia: Membrane separation
Institute on Membrane Technology, ITM-CNR, Italy: Novel composite membranes containing ionic liquid and selected polymers for specific gas/gas, gas/vapour and vapour/vapour separations
KIT Karlsruhe: Sulfur dioxide oxidation using heterogeneous catalytic microreactor
National Chung Hsing University, Taiwan: Preparation of Dense Homogeneous Polymeric Membranes and Study on Their Gas Permeation Properties
Otto von Guericke University of Magdeburg, Magdeburg, Germany: Mass transport through porous membranes

Procter&Gamble, Belgium: Research and development of new methods of emulsification using microtechnology
Slovak University of Technology in Bratislava, Slovakia: Processing of tall soap/oil extraction products
Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapours 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 vapour 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

Visits abroad

A. Heyberger: CSIR of Johannesburg, University of KwaZulu-Natal, Durban, South Africa (1 month)
J. Křišťál: Procter & Gamble, Brussels, Belgium (3 months)

Visitors

J. Aubin, CNRS Toulouse, France
M. Botha, University of KwaZulu-Natal, Durban, Republic of South Africa
A. Bucić-Kojić, Faculty of Food Technology, Osijek University, Croatia
M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
A. Palavra, Technical University of Lisbon, Portugal
S. Tigri, ENSIASET, Toulouse, France

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] Bouzek K., Jiřičný V., Kodým R., Křišťál J., Bystroň T.: Microstructured Reactors for Electroorganic Synthesis. (Eng) Electrochim. Acta 55(27), 8172-8181 (2010).
[2] Grosso C., Coelho J.P., Pessoa F.L.P., Fareleira J.M.N.A., Barroso J.G., Urieta J.S., Palavra A.F., Sovová H.: Mathematical Modelling of Supercritical CO_2 Extraction of Volatile Oils from Aromatic Plants. (Eng) Chem. Eng. Sci. 65(11), 3579-3590 (2010).

[3] Hanika J.: Mikroreaktory a vývoj nových technologií. (Czech) Microreactors and Development of New Technologies. Chem. Listy 104(7), 724-726 (2010).
[4] Hanika J.: 50. výročí založení Ústavu chemických procesů AV ČR, v. v. i. (Czech) 50th Anniversary of the Institute of Chemical Process Fundamentals of the ASCR, v. v. i. Chem. Listy 104(7), 738-739 (2010).
[5] Hanika J.: Chemie kolem nás. (Czech) Chemistry around us. Vesmír 89(10), 590-592 (2010).
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Fields of research

- Experimental determination and modelling of phase equilibria in fluid and condensed systems, including systems containing ionic liquids and systems with chemical reaction
- State and phase behaviour of fluids at superambient conditions (up to very high pressures)
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Molecular simulations of chemically reacting systems in nanoporous materials
- Mesoscale simulations of polymeric/nanoparticle systems and of energetic and reactive materials
- Development of molecular theory of polar and associating compounds (and their mixtures)
- Development of equations of state based on molecular theory
- Development and application of density functional theory for inhomogeneous fluids
- Hydrophobic interactions
- Percolation and nucleation
- Application of statistical-mechanical models to real fluids
- Thermodynamic modelling and processing of thermodynamic data

Applied research

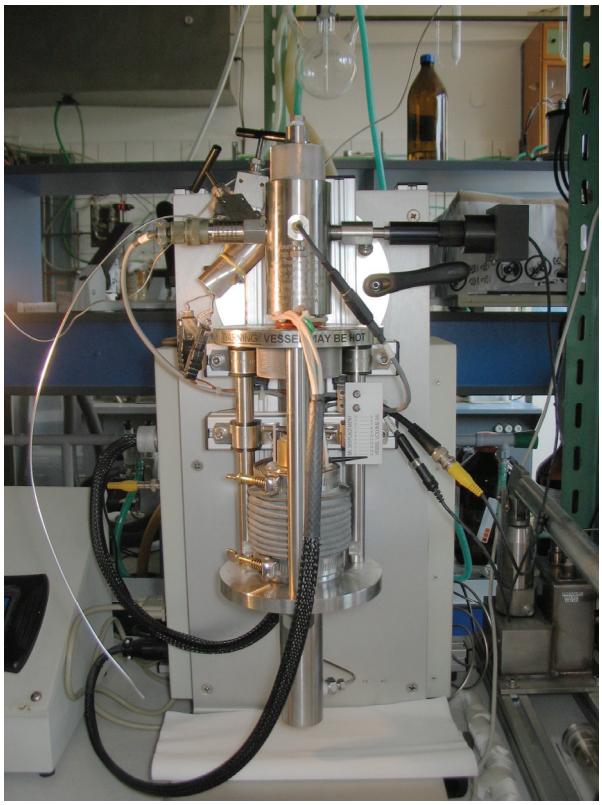
- Technology for preparation of molecularly imprinted polymeric materials

Research projects

Determination of the phase and state behaviour of fluids and fluid mixtures for processes at superambient conditions: molecular-based theory and experiment

(K. Aim, joint project with UJEP and CTU, supported by ASCR, grant No. IAA400720710)

Research was focused on application of results obtained in the framework of perturbation methods. The use is made of the finding that the inclusion of a short-range part of the total attractive interaction into a reference system allows a natural extension of the traditional first-order perturbation theory of simple fluids to practically all thermodynamic states. Research continued also on applications of the perturbation theory using a reference system based on the short-range part of intermolecular interactions to describe the thermodynamic behaviour of systems containing carbon dioxide + alkanols. Vapour pressures of a set of aliphatic alcohols were determined experimentally. The measurements of liquid-liquid equilibria in binary systems of 1-ethyl-3-methylimidazolium ethyl sulphate + C7 hydrocarbons were completed and the data obtained were successfully represented by polymer-solution models. [Refs. 1, 4-6, 8, 10, 15, 29, 32, 34, 38, 45, 51-54]



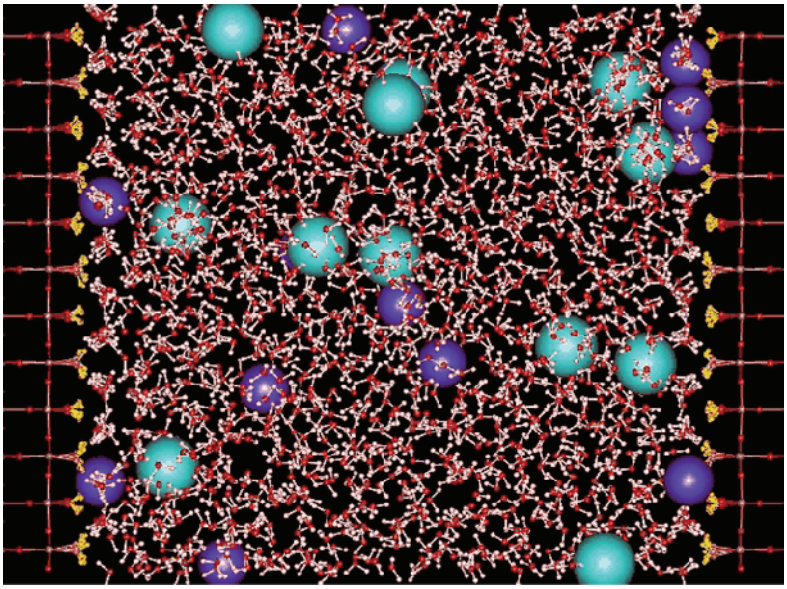
Variable-volume view cell (Super Phase Monitor SPM 20, Thar Technologies) for the determination of phase equilibria at high pressures

Computer modelling of structural, dynamical and transport properties of fluids in nanospace

(M. Lísal, joint project with University of South Bohemia in Ceske Budejovice, supported by GACR, grant No. GA203/08/0094)

Behaviour of fluids in the nanospace, solid-liquid interfaces (metal oxide-aqueous solution) and nanoporous carbons (activated carbons and carbon nanotubes) is studied by equilibrium and nonequilibrium molecular simulations to provide structural, dynamical and

transport properties of fluids in nanoconfinement. At solid-liquid interfaces, the simulation results for dynamics of water molecules are linked with quasielastic neutron scattering; the space-dependent shear viscosity and the dielectric properties are linked with electrophoretic data. We are also developing a method for the determination of local, space-dependent permittivity in inhomogeneous systems. In the case of nanoporous carbons, we adopt the methods for calculating local, space-dependent diffusivity and shear viscosity of pure fluids to slit and cylindrical nanopores, develop a method for the determination of space-dependent shear viscosity of fluid mixtures from computer simulations, and simulate the structural, dynamical and transport properties of industrially important fluid mixtures in carbon nanopores. [Refs. 11, 18-20, 22, 23, 26, 28, 35, 39, 46, 47]



Ions-water system in nanoslit with TiO_2 walls

EFCE Working Party "Fluid Separations"

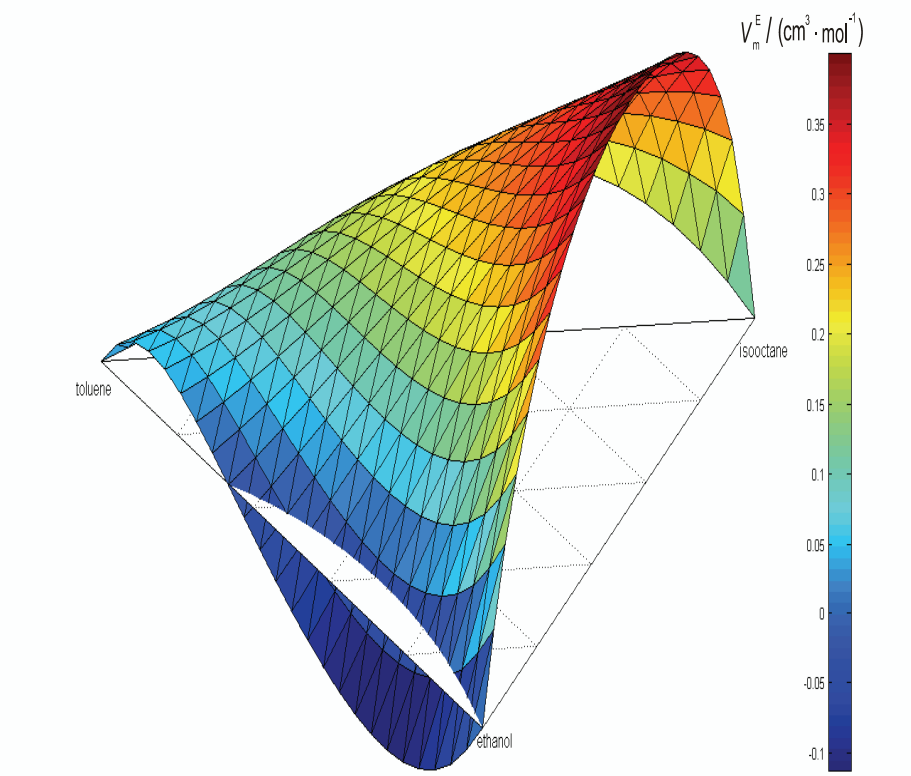
(M. Bendova, supported by MEYS, programme INGO project No. LA320)

Activities connected with membership of M. Bendova in EFCE Working Party on "Fluid separations". On behalf of M. Bendova, K. Machanova took part in the International Symposium on Solubility Phenomena in Leoben on July 25–30, 2010. [Ref. 31]

P-V-T behaviour of liquid mixtures constituting engine biofuels – experimental determination, correlation and prediction

(J. Linek, supported by GACR, grant No. GA104/09/0666)

Densities and sound velocities for binary systems composed of isooctane, toluene, and MTBE were measured at four temperatures within the range of 298.15 to 328.15 K at atmospheric pressure. Statistic and gnostic methods were applied to fit the incomplete data of excess volumes. Volumetric properties of pyridine, 2-picoline, 3-picoline, and 4-picoline at temperatures from 298.15 K to 328.15 K and at pressures up to 40 MPa were experimentally determined. Volumetric behaviour of ternary liquid system composed of ethanol, isooctane, and toluene at temperatures from 298.15 K to 328.15 K was also measured and correlated to determine the necessary number of ternary constants to fit the experimental data within experimental errors. [Refs. 13, 14, 41, 42]



Excess molar volumes (V^E_m) plotted against mole fraction of components (ethanol/isooctane/toluene) at T = 298.15 K and atmospheric pressure

Simple and complex models of aqueous solutions: The effect of nonadditive interactions

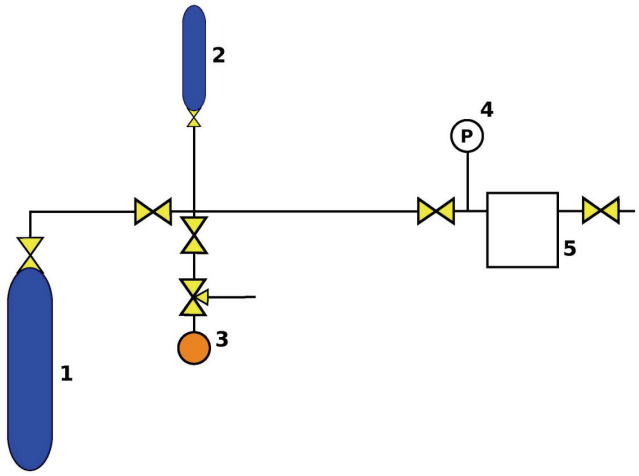
(I. Nezbeda, supported by ASCR, grant No. IAA400720802)

The multi-particle move Monte Carlo (MPM-MC) method developed in 2008 has been further extended and fully reviewed. An analysis of the behaviour of metastable water was carried out with two contradicting results, one from molecular simulations and the other from available equations of state. Exact expressions for the description of interaction of fluids at solid surface of variable curvature have been derived. [Refs. 7, 12, 15, 16, 21, 24, 25, 36, 37, 43, 44]

High-pressure phase equilibrium and p-V-T behaviour

(Z. Sedláková, supported by GACR, grant No. GP203/09/P141)

A new apparatus for measurement of high-pressure phase equilibria by synthetic method was assembled, based on Thar Technologies Super Phase Monitor. Accuracy of the apparatus was first checked by measuring the solubilities of supercritical CO_2 in ethanol, butanol, and 1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl] imide ([EMIM][TFSI]). New ternary high-pressure data have been obtained for system CO_2 + 1-butanol + [EMIM][TFSI]. For easy recyclability of ionic liquids, binary systems of amines and ionic liquids are investigated for use in carbon dioxide capture; solid-liquid and liquid-liquid equilibria in system diethylamine + [EMIM][TFSI] have therefore been studied. Experimental data were correlated by using the Redlich-Kister equation and compared with calculated ideal solubilities. Density and viscosity of ammonium-based ionic liquid were determined. [Refs. 14, 30, 31, 40-42, 48-50]

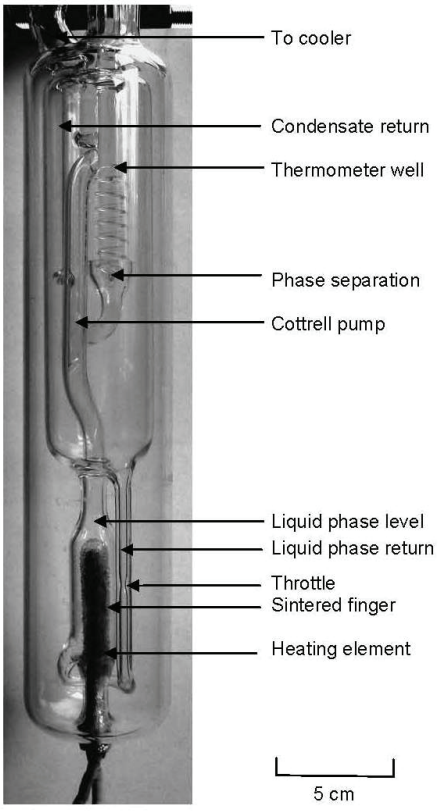


Assembly for the measurement of high-pressure phase equilibria: 1 - gas cylinder, 2 - CO_2 reservoir, 3 - vacuum pump, 4 - external pressure gauge, 5 - Super Phase Monitor SPM 20

Phase equilibria for the design of energy efficient separation processes

(I. Wichterle, supported by ICPF)

Vapour–liquid equilibrium data have been measured in binary and ternary systems of compounds with selected functional groups. New microebulliometer for total pressure measurement was developed, tested and used to measure the component activities in mixtures of polymers with organic solvents. A collection of data on miscibility and phase behaviour of binary polymer blends based on styrene, 2,6-dimethyl-1,4-phenylene oxide and their derivatives was published. [Refs. 2, 3, 9, 17, 27, 33]



New microebulliometer for total pressure measurement

International co-operations

INA, Research and Development, Zagreb, Croatia: Properties of polymer solutions
Institute of Condensed Matter, Ukrainian Academy of Sciences, Lviv, Ukraine: Modelling of molecular fluids at extreme conditions: Theory and applications
Institute of Physical Chemistry Ilie Murgilescu, Romanian Academy of Sciences, Bucharest, Romania: Phase properties of systems containing ionic liquids
Oak Ridge National Laboratory, Oak Ridge, TN, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems
Pennsylvania State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behaviour of model proteins on surface
Queen's University Ionic Liquids Laboratory (QUILL), Belfast, UK: Liquid-liquid phase equilibria in systems of ionic liquids
Technical University of Vienna, Austria: Colloids and theory of fluids
Université François Rabelais, Tours, France: Liquid-liquid phase equilibria in systems of ionic liquids
University of Ljubljana, Ljubljana, Slovenia: Water and hydration of nonpolar and ionic solutes
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

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)
K. Machanová: Laboratoire PCMB, Université François Rabelais, Tours, France (2 weeks)
A. Malijevský: Imperial College, London, UK (3 months)
Z. Sedláková: Laboratoire PCMB, Université François Rabelais, Tours, France (2 weeks)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

D. Gheorghe Chiscan, Institute of Physical Chemistry Ilie Murgilescu, Romanian Academy of Sciences, Bucharest Romania
J. Jacquemin, Laboratoire PCMB, Université François Rabelais, Tours, France
D. Lemordant, Laboratoire PCMB, Université François Rabelais, Tours, France
R. Melnyk, Institute of Condensed Matter Physics, Lviv, Ukraine
A. Trokhymchuk, Institute of Condensed Matter Physics, Lviv, Ukraine
V. Vlachy, University of Ljubljana, Ljubljana, Slovenia

Teaching

K. Aim: ICT, Faculty of Chemical Engineering, postgraduate courses "Experimental methods of determination of phase equilibria in fluid systems" and "Applied statistical analysis and processing of data"

M. Bendová: ICT, Faculty of Chemical Engineering, postgraduate course "Physical chemistry for technological practice"
J. Jirsák: UJEP, Faculty of Science, courses "Physical Chemistry Seminar", "Essential of programming languages"
M. Kotrla, M. Předota: CU, course "Advanced computer simulations in many particle systems"
M. Lísal: ICT, Faculty of Chemical Engineering, postgraduate course "Physical chemistry for technological practice"
M. Lísal: UJEP, Faculty of Science, courses "Parallel programming", "Numerical Mathematics I" and "Numerical Mathematics II"; tutorials "Molecular Simulations I"
I. Nezbeda: UJEP, Faculty of Science, courses "Molecular simulations I", "Principles of Scientific Communication" and "Statistical Physics"
I. Nezbeda, K. Aim: ICT, Faculty of Chemical Engineering, postgraduate course "Applied statistical thermodynamics of fluid systems"
M. Předota: University of South Bohemia, Ceske Budejovice, courses "Lectures from physics oriented to particle and nuclear physics" and "Selected lectures from physics"

Publications

Original papers

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Slovak Society of Chemical Engineering, Proceedings, p. 171, Tatranské Matliare, Slovakia, 24-28 May 2010.

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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 of porous solids
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Transport processes in porous solids
- Unconventional preparation of supported molybdenum catalysts
- Preparation and characterization of electrospun nanofibrous membranes

Applied research

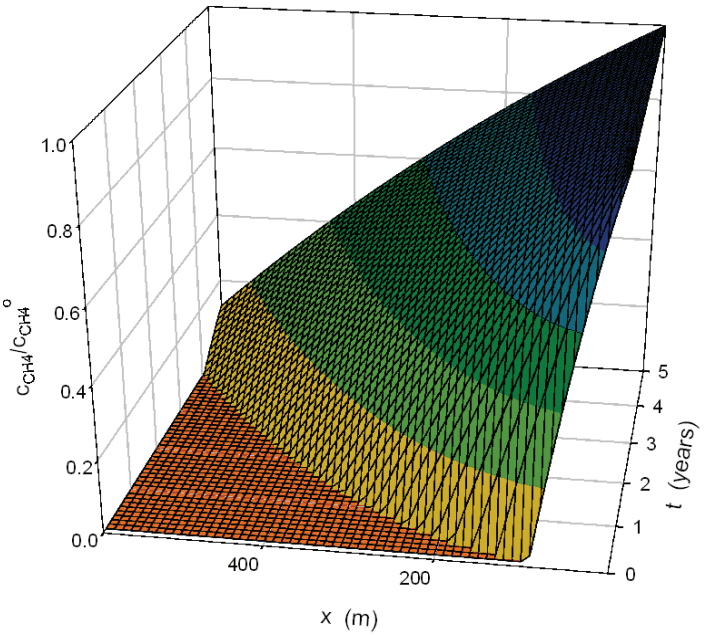
- Catalytic combustion of volatile organic compounds
- Esterification of free fatty acids in low-cost raw materials for biodiesel production
- Oxidation processes for environment
- Textural characteristics of structural materials

Research projects

Hydrogen oriented underground coal gasification for Europe

(O. Šolcová, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00006)

Project explores technology for hydrogen production through underground gasification of coal in a dynamic geo-reactor. Process is controlled through purposed dynamic changes in temperature and pressure of the reactants and products. The project addresses CBM usage and CO_2 sequestration in coal deposits. The environmental fingerprint of the technology on air, water and strata stability is evaluated. Locations of demonstration plants are chosen through computer modelling and simulation. Large scale production of hydrogen from coal is crucial for coal mining industries and will serve the needs of energy, chemistry and transportation sectors of Europe. [Refs. 27, 47, 110-112]

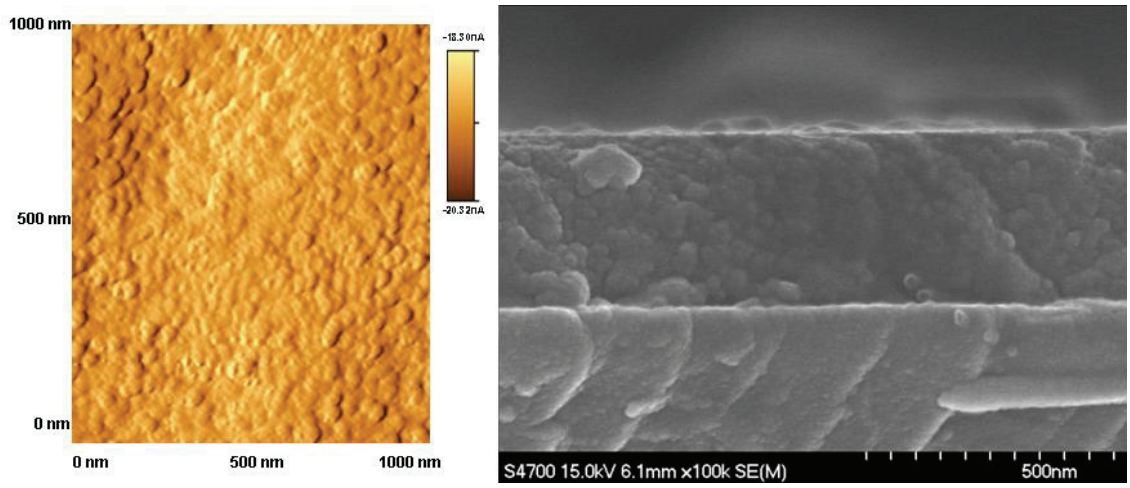


Gas transport through the porous stratum

Hierarchic nanosystems for microelectronics

(O. Šolcová, joint project with JH IPC, IMC, Institute of Microbiology of the ASCR, v. v. i., Institute of Physics of the ASCR, v. v. i., ICT, CU, UJEP, and Research Institute of Organic Syntheses Pardubice, supported by ASCR, project No. KAN400720701)

Project develops the complex composite systems with precisely defined performance applicable in microelectronics. The individual components are formed by small arranged particles which ensure partial function inevitable for functioning of the whole system. These composite structures should be directly applicable as elements of special sensors, photoelectric energy sources, microelectrodes for analytic instruments etc. The general aim of the project is the accumulation of sufficient amount of high-quality experimental data to be applied for design and implementation of practical nanotechnologies. Professionally, this project is focused on the study of preparation of hierarchic nanostructures, inclusive the structural and functional characterization, as well as on prediction of properties by means of mathematical modelling. [Refs. 5, 13-15, 21, 31, 37, 43, 73, 82, 95, 100]



Detail of a sensor surface

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

(O. Šolcová, joint project with Dekonta, a.s., supported by MIT, grant 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 waste by the thermal desorption process and a 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. [Refs. 10, 12, 48, 50, 51, 80, 81, 115]

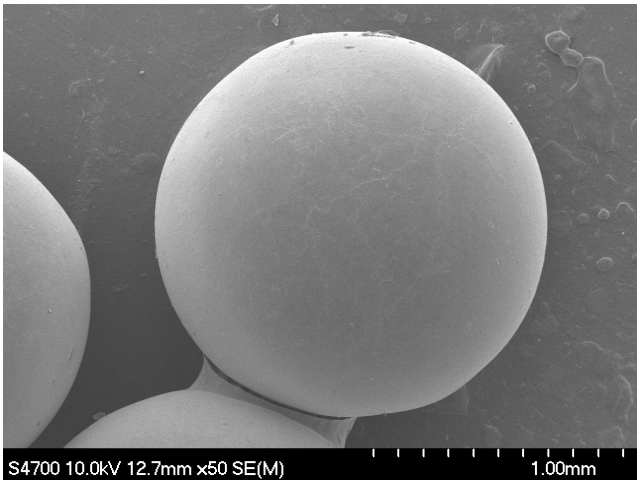
Pilot unit for catalytic oxidation of desorbed organic contaminants

Advanced photocatalytic processes - nanotechnology for environment

(O. Šolcova, joint project with Institute of Microbiology of the ASCR, v. v. i., and UPCE, supported by GACR, grant No. GA104/09/0694)

This project is focused on preparation and characterization of specially designed photo-active materials and their utilization for decomposition of a large series of potential water contaminants ranging from phenols, chlorinated phenols, polybrominated diphenyl ethers and alcohols to herbicides, pesticides, pharmaceuticals, industrial colourants, pigments and dyes. The special focus is devoted to design the reactor system; selectively prepared photo-active

nanostructures together with design the effective photoreactors including mathematical modelling of involved physical and chemical processes and generalization of obtained results. [Refs. 3, 11, 19, 36, 89, 91, 101, 116]



Supported titania nanocrystals for water treatment

Advanced catalytic processes and materials

(J. Hanika, O. Šolcová, joint project with JH IPC, ICT, CU, and UPCE, supported by GACR, grant No. GD203/08/H032)

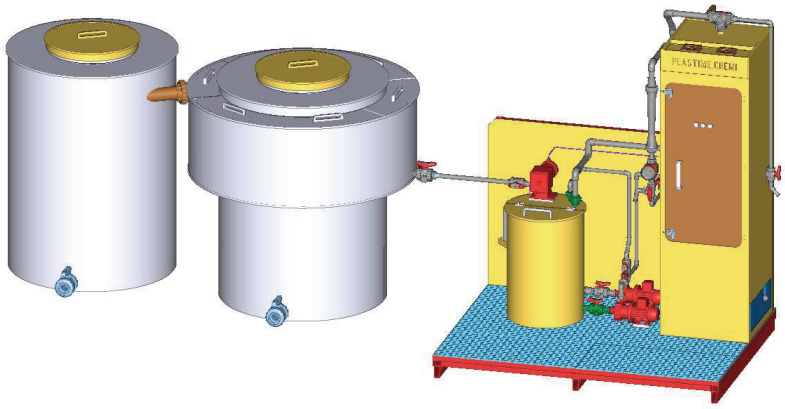
This project is aimed at development of the new selective catalytic and separation processes for preparation of special compounds and materials which can give progression in the field of the new chemical technologies. Processes in question are stereoselective and regioselective transformations on chiral catalytic centres and processes with significant environmental impact. Coordination of thesis projects is planned in the field of catalysis, e.g., developed Rh catalysts can be tested in stereospecific polymerizations (CU), asymmetric synthesis (ICT) and hydrocarbonylations; oxidation catalysts can be tested in organic synthesis (ICT, UPCE, ICPF), oxidation polymerization (CU) and synthesis of chemical specialties (JH IPC); new mesoporous materials prepared at JH IPC will be used in all other partner laboratories, etc. [Refs. 18, 23, 38, 44, 46, 61, 62, 83-85, 90, 92, 93, 102, 117, 118]

Newly designed nanoadsorbents for photocatalysis

Reactive chemical barriers for decontamination of heavily polluted waters

(P. Klusoň, joint project with Dekonta a.s., supported by MIT, grant No. FR-TI1/065)

This project aims at the practical development of special oxidation processes used for decontamination of industrially polluted subsurface waters. The used methods are: photocatalytic oxidation with titanium dioxide, photocatalytic oxidation with synthetic porphyrines and oxidations with various organic peroxides and hydrogen peroxide. The project deals in a complex manner with the problem of industrial pollution with a range of organic chemicals at concentrations and the area scale that can hardly be treated in any other way. The Recheba concept represents a kind of passive approach, however, assisted with highly advanced processes for effective water decontamination. The systems are now tested on a laboratory scale, in parallel they will be modified and scaled-up for practical testing on three selected industrial sites. The efficiencies of the chosen methodologies will be compared and the most suitable one will be implemented to the final form that will be produced and long-term tested. [Refs. 24, 30, 52, 53, 59, 68]

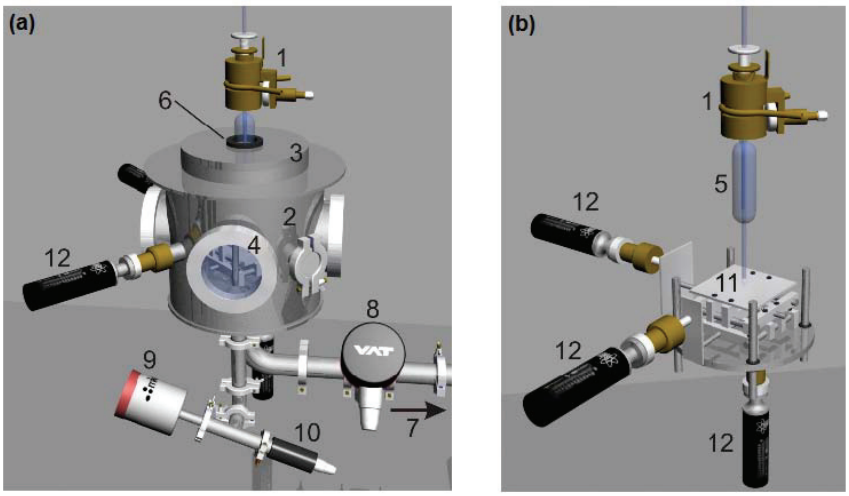


Scheme of the chemical barrier decontamination system

Composed molecular templates for preparation of assembled functional nanoparticles

(P. Klusoň, bilateral project with Bangor University, School of Chemistry, Wales, UK, supported by ASCR, grant No. M200720904)

To emulate at least some of the effectiveness of NATURE in making smart functional structures and systems man has had to develop many different empirical and later also scientific concepts. Currently such attempts are reflected in the steep growth of interest in nanoscience and nanotechnologies. Although there has already been much progress in the synthesis, assembly and fabrication of nanomaterials, their potential applications in a wider range of practical technologies are still rare. These new technologies are expected to have an impact on chemistry, energy production, energy storage, electronics, machinery, aircrafts, space exploration, environment protection, etc. Independently of types of new materials (or their application), one of the most important points concerns chemical (or physical) pathways that are capable to yield them. Among the suitable 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. [Refs. 6, 16, 17, 49, 54, 60, 63, 103]

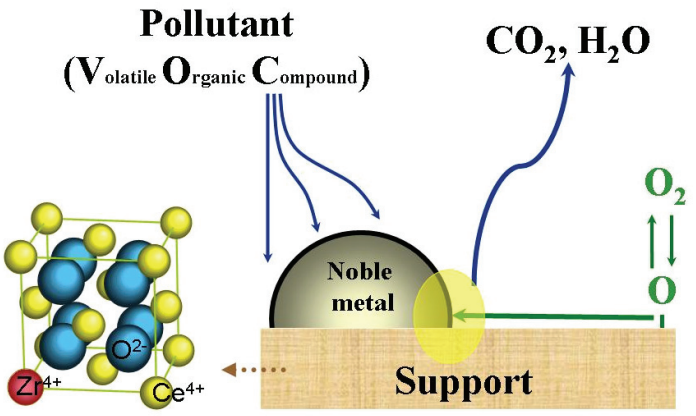


Experimental set-up: (a) surfatron plasma source, (b) inside facility of the chamber

New catalysts for VOC oxidation

(J. Gaálová, joint project with Department of Process and Environmental Engineering, University of Oulu, Finland, supported by ASCR, grant No. M200720901)

The aim of this project is development of catalyst for oxidation of the volatile organic compounds (VOCs) based on noble metals. Ceria-zirconia mixed oxides attracted special attention due to their unique property of storing and releasing oxygen and excellent thermal and mechanical resistance. Platinum catalysts supported on Ce-Zr mixed oxides that were recently developed in this project exhibited comparable performance to commercial catalysts even with lower Pt loading. On the other hand, gold supported on Ce-Zr mixed oxides proved better selectivity to CO_2 than its platinum and commercial analogues, with activity being only slightly worse. Tailored synthesis of monolithic catalysts based on these systems will be studied in near future. [Refs. 42, 65, 114]



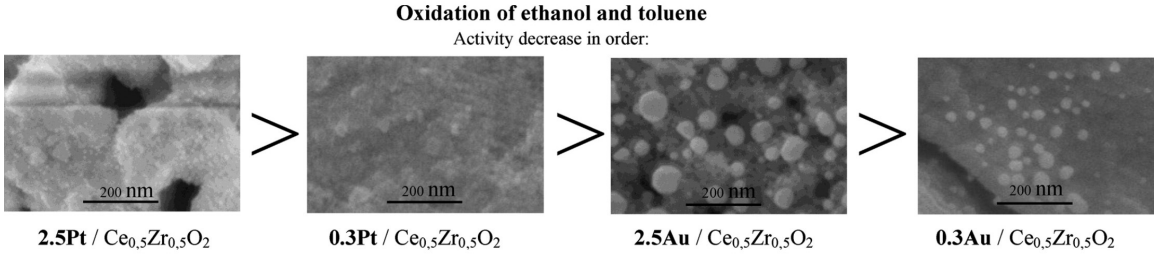
The Ce-Zr mixed oxide as support for noble metal in oxidation of VOC

Development of oxide catalysts for total oxidation of ethanol

(J. Gaálová, supported by GACR, grant No. P106/10/P019)

This project is focused on development of catalysts with higher activity and selectivity for ethanol oxidation to CO_2 than those studied previously. Importance of the project contributions is underlined by taking advantages from analogies between ethanol and other volatile organic compounds (VOC), and multiple the use of those materials. The research

investigates the expansion of information about activity of mixed oxide based catalysts and effect of their promoters in VOC oxidation. Project clarifies selectivity of the catalytic materials. Predications of the new directions about their preparation and composition are formulated, which could helps to solve important environmental problem. [Refs. 34, 66, 106]

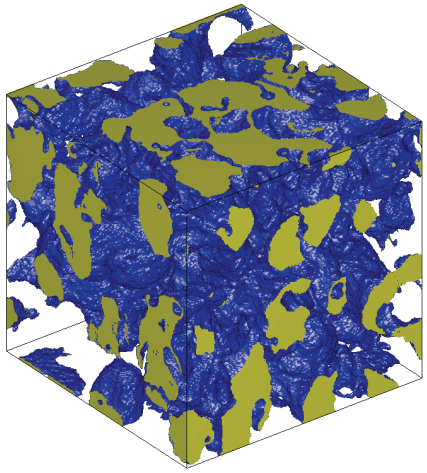


Activity of the Ce-Zr mixed oxides as supports for Pt and Au in oxidation of ethanol and toluene

Routes to separation performance enhancement for composite membranes based on linear polyimides

(V. Hejtmánek, joint project with JH IPC and ICT, supported by GACR, grant No. GA203/09/1353)

Aromatic polyimides (PI) exhibit very good chemical and mechanical stability up to 250 ºC. They also exhibit a high selectivity for membrane separation of small molecules as hydrogen. The main drawback PI membranes preventing their wide application, e.g. in membrane reactors is a very low species flow. The principal goal of the project is thus, enhancement of species flow without essential deterioration of the selectivity. The approaches considered to enhance species flow through membranes are: (i) thinning of the PI layer upon introducing porous supports or armour, (ii) formation of PI layer upon radial stress, (iii) producing local stress fields by introducing inclusions, (iv) introducing porous inclusions at concentrations near to percolation threshold. To optimize two-phase membrane composition, it is intended to perform a rigorous treatment of mass transport in composite media using image analysis together with computer experiment. [Refs. 2, 57, 58, 64, 69, 70]

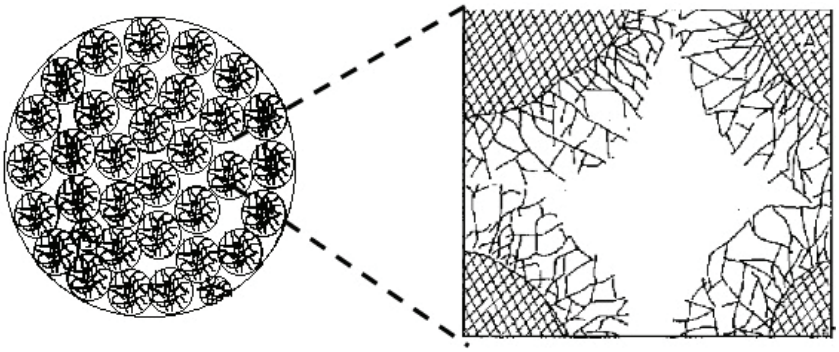


The zeolite-polyimide membrane replica (64×64×64 μm). Polyimide phase is transparent, polyimide-silicalite interface is blue and intersections of the silicalite phase and the cut planes are yellow

Functional macroreticular polymers as catalyst carriers

(K. Jeřábek, joint project with Department of Chemical Sciences, University of Padua, Italy, supported by ASCR, grant No. M200720902)

In the project, polymer-based catalysts bearing either covalently bonded acidic groups and/or metal nanoparticles are investigated. Using combination of various physico-chemical methods, morphology and steric conditions in polymeric catalysts of both laboratory and commercial origin has been examined. Methods for modification of porous structure of functional polymers by additional post polymerization cross-linking were also studied. In starting stages is the investigation of modification of chemical nature of polymer catalyst carriers for applications in highly lipophilic environment. [Refs. 7, 28, 71, 72, 74, 75]

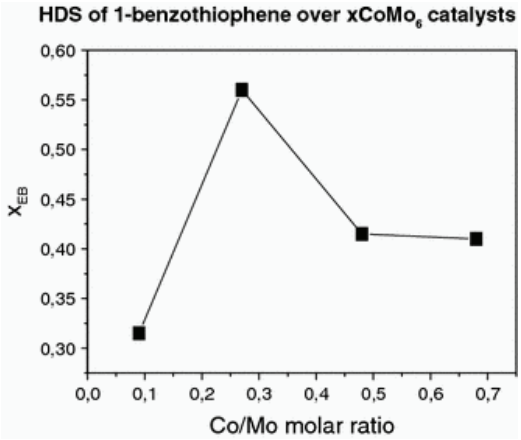


Schematic depiction of macroreticular polymer morphology

Synergistic effects in hydrodesulfurization and oxidation reactions

(K. Jirátová, bilateral co-operation with Institute of Catalysis, BAS, Sofia, Bulgaria, supported by ASCR)

The effect of cobalt amount on hydrodesulfurization activity of Al_2O_3-supported hetero-molybdate was studied, as well as the effect of various supports (TiO_2-ZrO_2 mixtures, tungsten-modified SBA-15 and HMS). [Refs. 20, 25, 29, 33]



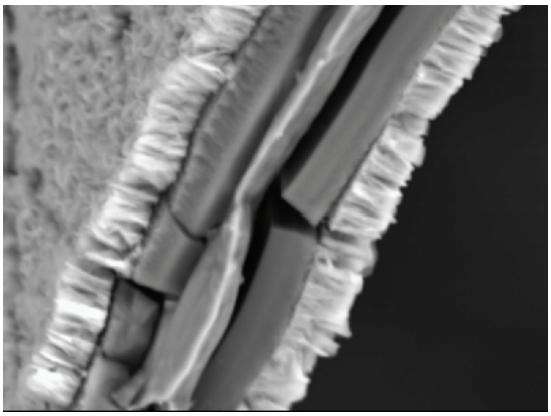
Effect of Co on HDS activity of alumina-supported heteropolymolybdate

Deposition of oxide catalysts for oxidation of VOC onto preformed support and their modification by nanoparticles of noble metals

(K. Jirátová, joint project with ICT, and IIC, supported by GACR, grant No. GA104/07/1400)

Binary and ternary Cu, Co, Ni, Mn/Al mixed oxides prepared by calcination of co precipitated LDH precursors were examined in total oxidation of ethanol. Formation of the

chosen LDH precursors on an oxidized Al foil, a model of structured catalyst supports, under hydrothermal conditions was studied in detail and after their calcination, activity of the resulting mixed oxides in ethanol oxidation was also examined in detail. [Refs. 35, 39, 40, 76, 77, 86-88, 94, 105]

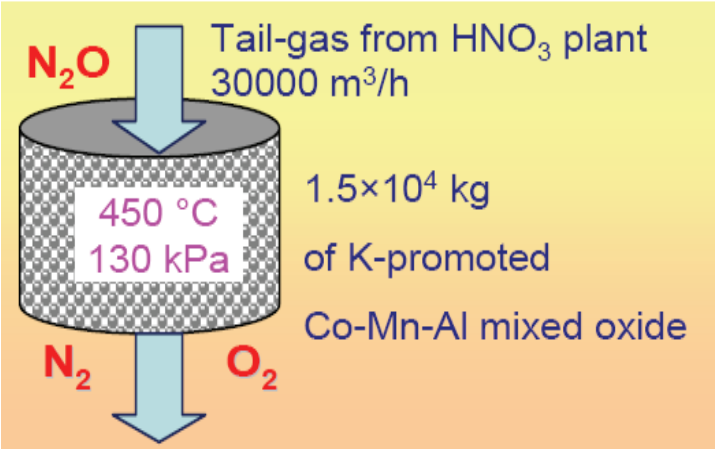


SEM of Co-(Mn)-Al catalyst precursor of LDH type grown on an oxidized Al foil

Supported oxidic catalysts containing low amount of active species as catalysts for N_2O decomposition

(K. Jirátová, joint project with TU of Ostrava, and ICT, supported by GACR, grant No. GA106/09/1664)

The effect of promoter addition to the calcined Co-Mn-Al LDH-like compounds on the catalyst activity in decomposition of N_2O was studied. Potassium was found to be the best promoter of the catalyst. Abatement of N_2O in waste by its decomposition over K-promoted Co-Mn-Al mixed oxide catalyst was simulated. [Refs. 9, 104]



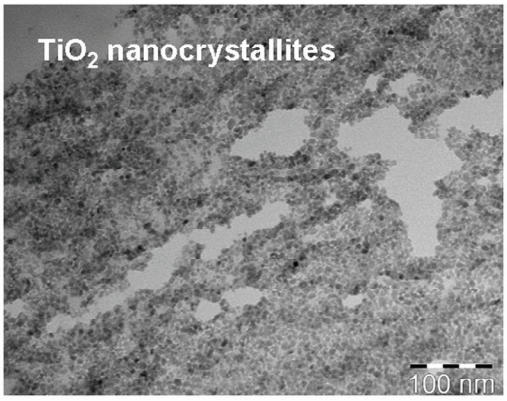
A K-promoted Co-Mn-Al mixed oxide catalyst derived from a layered double hydroxide (LDH)

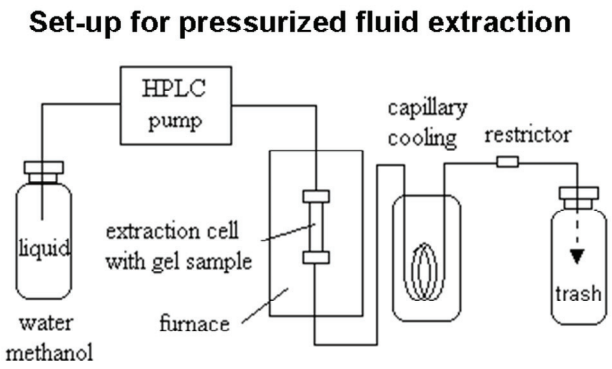
Innovative preparation of nanocrystalline metal oxides with high-ordered mesoporous structure by extraction technique

(L. Matějová, supported by GACR, grant No. GP104/09/P290)

Project deals with development and optimization of extraction technique for purification and total crystallization prepared oxidic materials with high-ordered mesoporous structure. Developed extraction technique using fluids in supercritical and subcritical state was

generally applicable for synthesis of nanocrystalline metal oxides. The optimal experimental conditions (temperature, pressure, flow rate, etc.) as same as the suitable solvents were defined and evaluated also with respect to future technical and economic realization of methodology. High-ordered mesoporous metal oxides (hexagonal, cubic, lamellar) TiO_2, ZrO_2, SiO_2/TiO_2, ZrO_2/TiO_2, CeO_2, Nb_2O_5, Ta_2O_5, SnO_2 promising in photocatalysis and sandwich structures in microelectronic were synthesized by templating using amphiphilic and ionic surfactants in aqueous and alcoholic solution with metal chloride and alkoxide. [Refs. 22, 41, 96-99, 113]



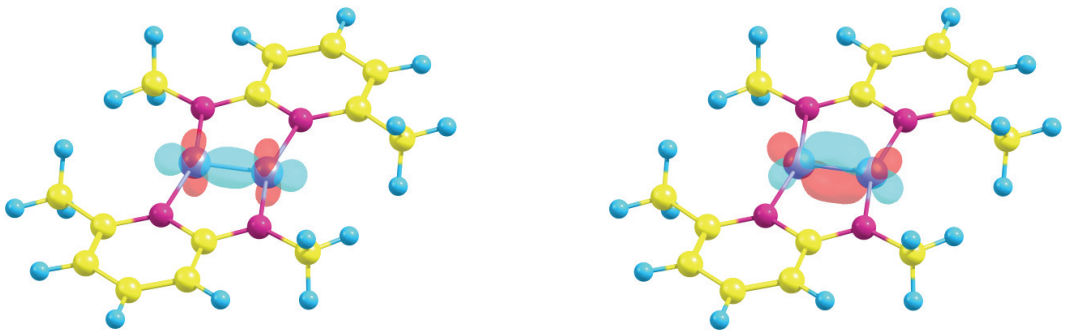


TiO_2 nanocrystallites; set-up for pressurized fluid extraction and purification

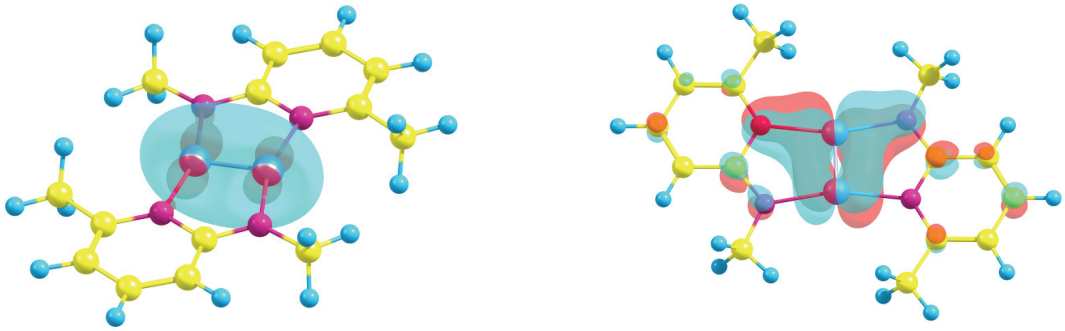
Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, supported by GACR grant 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 behaviour 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 bond. Especially useful in this respect were found the approaches known as the analysis of domain-averaged Fermi holes (DAFH) and the generalized population analysis. These approaches have been applied to the interpretation of the bonding in molecules with complicated bonding pattern like metal-metal bonding, multicentre bonding, all metal aromaticity, etc. The formalism of the analysis of domain averaged Fermi holes was generalized beyond the scope of closed shell systems and the attention was also paid to the manifestation of the chemical bonding in momentum space. [Refs. 1, 4, 26, 45, 55, 56, 107-109]



a) 0.982 b) 0.996



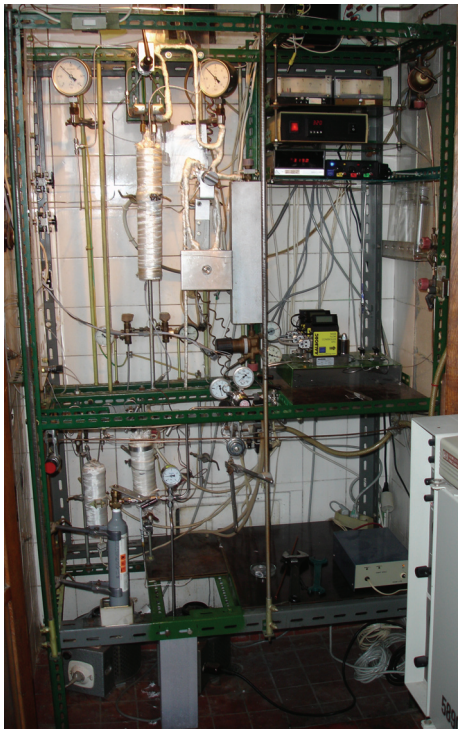
c) 0.928 d) 0.909

Results of DAFH analysis for the studied complex with multiple Cr-Cr bond. Selected eigenvectors (and associated eigenvalues) of the Fermi holes corresponding to broken valences of Cr-Cr bond for the holes averaged over the domain involving one Cr atom respectively

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

(Z. Vít, supported by GACR, grant No. 104/09/0751)

Alternative supports and active phases for hydrodesulfurization (HDS) were studied. Mesoporous silica-aluminas modified by acid extraction were studied as supports of Pt and Pd catalysts. The extraction led to higher surface areas and Brønsted acidities of supports which improved the HDS activity of Pt and Pd catalysts. Rh sulfide deposited on different alumina supports and CoMo catalysts prepared from the heteromolybdate precursors were studied in HDS of thiophene. The HDS and hydrogenation activities of different transition metal sulfides deposited on alumina, titania and zirconia were studied in reactions of benzothiophene and 1-methylcyclohexene. Inhibition effect of pyridine on HDS of thiophene was studied on Rh and Ru promoted Mo/alumina catalysts. [Refs. 8, 32, 67, 78, 79, 119, 120].



Microreactor with fixed bed of catalyst

International co-operations

Bangor University, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials
Catholic University of Louvain, Louvain-la-Neuve, Belgium: Development of VOC oxidation catalysts
Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
Chemistry department, University of Pecs, Hungary: visualization of the bonding interactions in transition metal complexes
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
Department of Physical chemistry, Slovak Technical University Bratislava, Slovakia: visualization of bonding interactions in transition metal complexes
European Membrane Institute, Montpellier, France: Synthetic porphyrites
Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia: Morphology of Poly-HIPE materials
Institute of Catalysis, Sofia, Bulgaria: Synergistic effects in hydrodesulfurization and oxidation reactions
Institute of Computational Chemistry, University of Girona, Girona, Spain: Theory of chemical bond
Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials
Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Visualization of bonding interactions in transition metal complexes
Institut Scientifique de Service Public, Liege, Belgium: Transport characteristics for coal gasification
Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification
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
University of Kragujevac, Serbia: Multicentre bonding, quantitative characterization of aromaticity
University of Liverpool, Liverpool, United Kingdom: Theory of chemical bond
University of Oulu, Oulu, Finland: New catalysts for VOC oxidation
University of Paris VI, Paris, France: Theory of chemical bond
University of Poitiers, Poitiers, France: New catalysts for VOC elimination
University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix
University of Udine, Udine, Italy: Characterization of noble metal catalysts
University of Vigo, Vigo, Spain: Multicentre bonding, theoretical characterization of aromaticity

Visits abroad

P. Krystynik: Bangor University, Bangor, Wales, United Kingdom (2 months)
L. Matějová: University of Oulu, Oulu, Finland (2 months)

Visitors

M. Boaro, University of Udine, Italy
R. Brahmi, University of Chouaib Doukkali, Morocco
L. Bučinský, Slovak Technical University Bratislava, Slovakia
B. Corain, University of Padua, Italy
O. Dudarko, Institute of Surface Chemistry NAS, Ukraine
P. Hudec, Slovak Technical University Bratislava, Slovakia
S. Ojala, University of Oulu, Finland
J. Penttinen, University of Oulu, Finland
S. Pitkäaho, University of Oulu, Finland
A. Spojakina, Institute of catalysis, Sofia, Bulgaria
Y. Zub, Institute of Surface Chemistry NAS, Ukraine

Teaching

F. Kaštánek: ICT, Faculty of Chemical Engineering, postgraduate course "Application of chemical engineering in technologies for environment"
P. Klusoň: ICT, Faculty of Chemical Engineering, postgraduate course "Physical chemistry for technological practice"
P. Klusoň, UJEP, Faculty of Environment, course "Toxicology"
R. Ponec: CU, Faculty of Science, course "Structure and reactivity"
O. Šolcová: ICT, Faculty of Chemical Engineering and Faculty of Chemical Technology, postgraduate course "Texture of porous solids"

Publications

Original papers

[1] Bultinck P., Cooper D.L., Ponec R.: The Influence of Atoms-in Molecules Methods on Shared Electron Distribution Indices and Domain Averaged Fermi Holes. (Eng) J. Phys. Chem. A 114(33), 8754-8763 (2010).
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[12] Kaštánek F., Šabata S., Šolcová O., Maléterová Y., Kaštánek P., Bránykiová I., Hetflejš , Zachleder V.: In-Field Experimental Verification of Cultivation of Microalgae Chlorella sp. Using the Flue Gas from a Cogeneration Unit as a Source of Carbon Dioxide. (Eng) Waste Manage. Res. 28(11), 961-966 (2010).
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Department of Multiphase Reactors

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MAREK RŮŽIČKA

DEPUTY
MÁRIA ZEDNÍKOVÁ

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TECHNICAL STAFF
STANISLAVA NOVÁKOVÁ

Fields of research

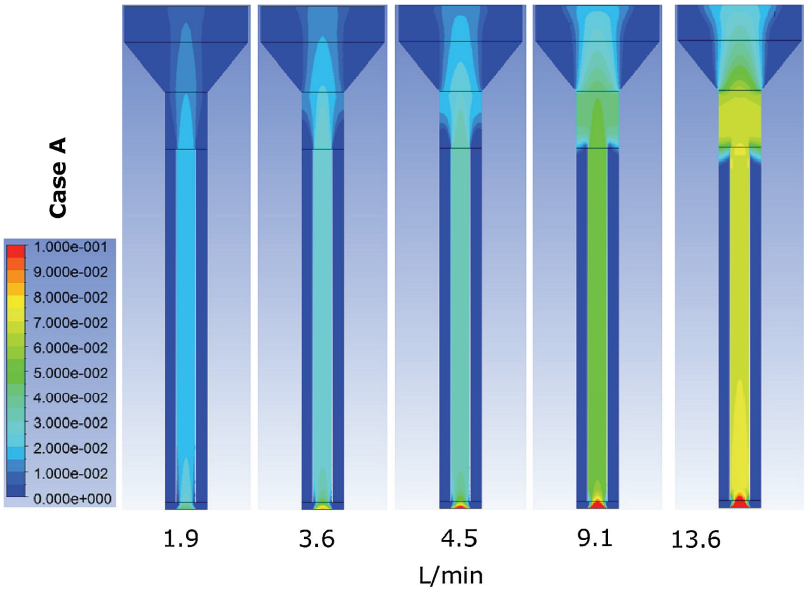
- Multiphase fluid dynamics and transport phenomena in different types of gas-liquid, liquid-solid or gas-liquid-solid systems
- Sedimentation of ensembles of polydisperse particles, deposit structure
- Flow of microdispersions and liquids with complex rheological behaviour
- Electrodiffusion diagnostics of the flow

Research projects

Hydrodynamics and transport phenomena in multiphase systems: from microscale to macroscale

(M. Růžička, joint project with TU of Ostrava, supported by GACR, grant No. GA104/07/1110)

Essence of the research project is the investigation into the basic physical mechanisms involved in hydrodynamics and transport phenomena in complex multiphase systems. Transport of mass and momentum in both two-phase systems (gas-liquid) and three-phase systems (gas-liquid-solid) were studied. The stress is put on the momentum transfer between the phases, i.e. on the hydrodynamics of multiphase flows. Hand in hand with the understanding the multiphase motion, the mass transfer phenomena were explored. The typical feature of the multiphase systems is the existence of a microstructure, given by the presence and configuration of the dispersed particles. The microstructure has a multi-scale nature and determines the system rheology. The project is aimed at resolving the relation between the microstructure and the macroscopic behaviour of the multiphase systems. [Refs. 4, 5, 7, 11, 14-16, 22, 24, 29, 32, 36-39, 54, 55, 58, 59]



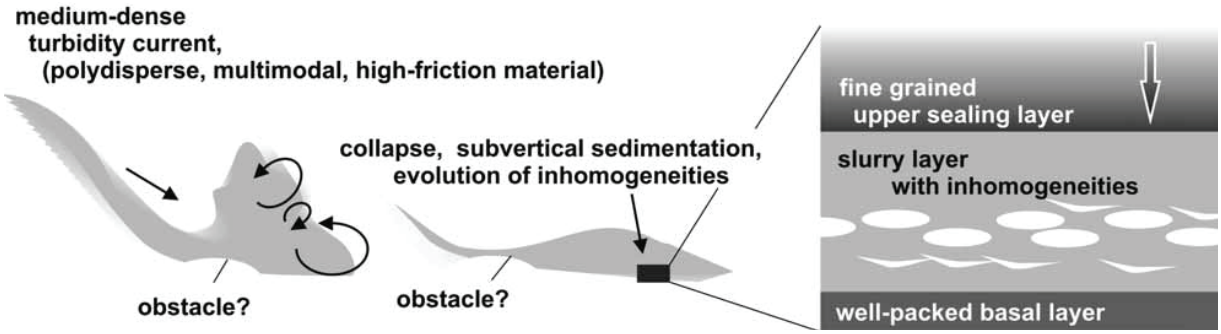
Case A simulations: Gas holdup fields for gas flow rates 1.9, 3.6, 4.5, 9.1, and 13.6 l min^{-1} (riser gas superficial velocity 1.0, 2.0, 2.5, 5.0, 7.5 cm s^{-1})

Hydrodynamic concept of stromatactis formation in geology

(M. Růžička, joint project with Institute of Geology of the ASCR, v. v. i., supported by ASCR, grant 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 inter-

disciplinary study is novel, and the results are fundamental for sedimentology and hydrodynamics, with possible implications in related technologies. [Refs. 14, 24]

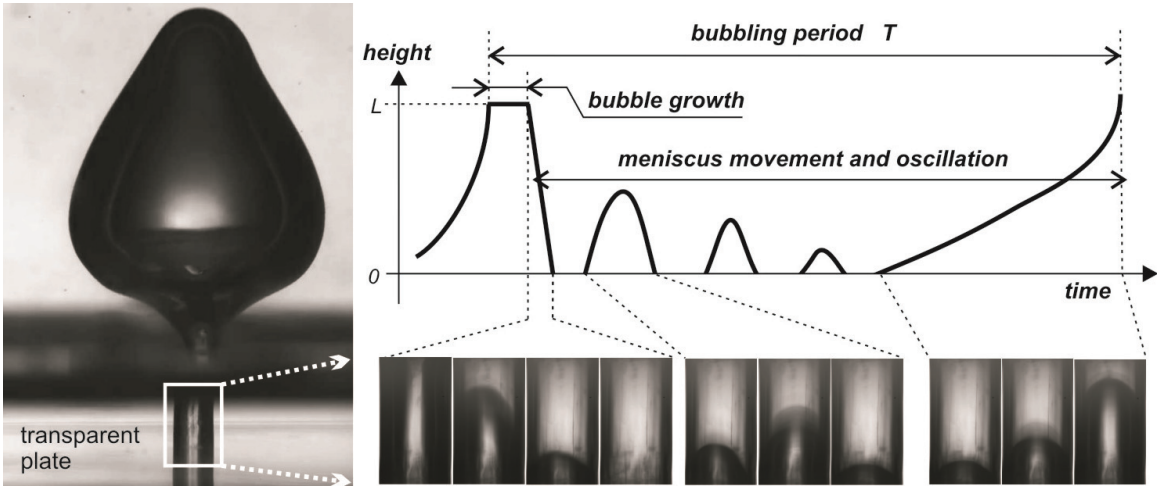


Event-sediment scenario for stromatactis-bearing beds

Dynamics of bubble formation at submerged orifices: Simultaneous formation and synchronous regimes

(P. Stanovský, supported by ASCR, grant No. KJB200720901)

A goal of this project is an experimental study of the dynamics of interfacial meniscus inside an orifice during bubble formation from a submerged orifice. Incorporation of the meniscus dynamics into a mathematical model of the bubble formation allows explaining aperiodicity in the bubble formation at one orifice. The project objectives are the experimental verification of the model in a wide range of parameters coupled with the study of interactions between external acoustic source and the meniscus motion. Finally, an extension of the model from one orifice to more orifices are done in order to explain a mechanism leading to an asynchronous regimes appearance during bubble formation at more orifices as well as an acquirement of new experimental data about simultaneous formation at multi-orifice spargers. [Refs. 4, 36-38]

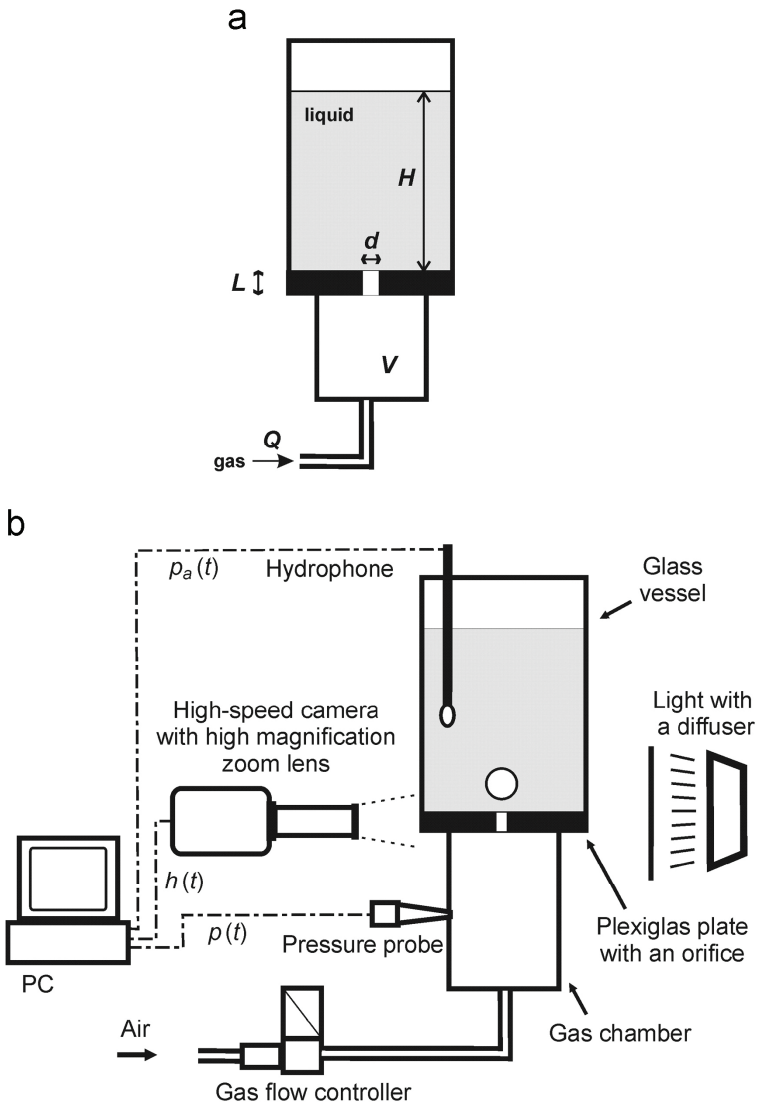


The studied key phenomena - *meniscus oscillation* - influencing the bubble size variability and bubble formation synchronicity at multiple orifices

Transport and reaction processes in complex multiphase systems

(J. Drahoš, joint project with ICT and UPCE, supported by GACR, grant No. GD104/08/H055)

Project is focused on training of doctoral students in the field of chemical engineering via targeted research in modern branches of chemical, pharmaceutical, biological and process industries with emphasis on research in new areas such as micro- and nanotechnologies and material engineering. It includes theoretical and experimental work of 20 students of Chemical Engineering Departments at ICT and UPCE, and at ICPF. Particular research programmes involve 16 areas from microsystems to industry-scale processes. Project is led by 18 supervisors. The training includes both general courses on mathematical modelling, statistical analysis and methodology of scientific work, and courses specialized on specific research fields. Students take part in national and international projects of cooperation with major research laboratories. The project output are publications in impacted international journals, presentations at conferences and special workshops with lectures by students, supervisors and invited specialists, published in proceedings. [Refs. 11, 14, 18-20, 22-24, 26-28, 50, 51]



Schematic diagram of the experimental apparatus: (a) measuring cell and (b) complete set-up

Presidency of the European Federation of Chemical Engineering (EFCE)

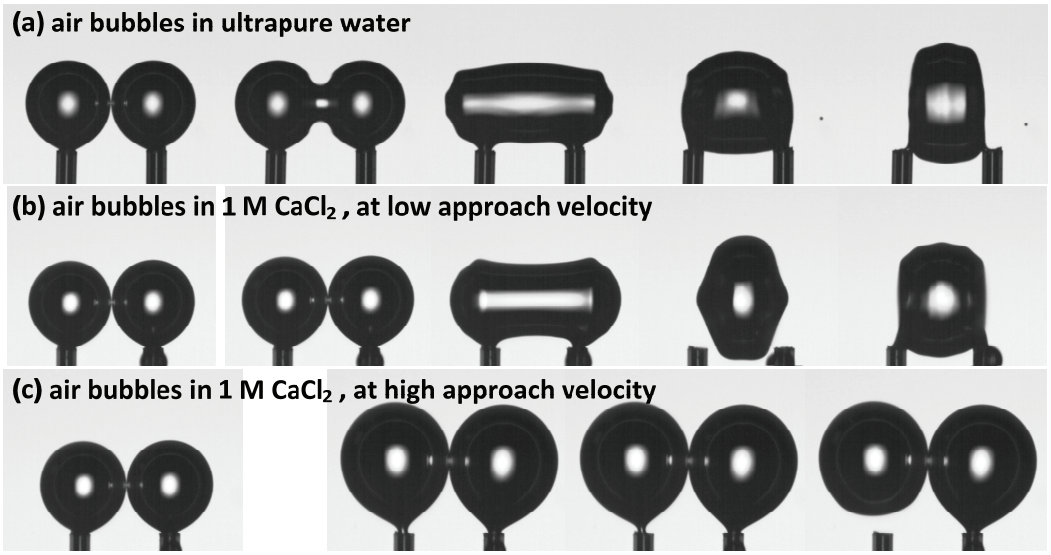
(J. Drahoš, supported by MEYS, INGO project No. LA 319)

The EFCE is one of the most important institutions in the field of chemistry. Prof. Jiří Drahoš successfully served for four years as its President for the period 2006-2009. Together with Prof. Růžička, he also participated at the activities of the EFCE Working Party Multiphase Fluid Flow. [Ref. 21]

Determination of the coalescence efficiency of bubbles in liquids

(S. Kordač Orvalho, supported by GACR, grant No. GP104/09/P255)

The coalescence phenomenon is of capital importance in the design and performance of multiphase contactors. Although studied for several decades, it is still not completely understood. The present project aims to improve our knowledge on the subject in the following way: to determine experimentally a relation between coalescence efficiency and the crucial control parameters (bubble properties, liquid properties, liquid flow conditions). Bubble coalescence was studied experimentally in a laboratory cell (pairwise first, multiple then) under well-defined conditions. Then, these small scale data have been related to the coalescence in real gas-liquid dispersions in bubble column reactors. [Refs. 29, 30]

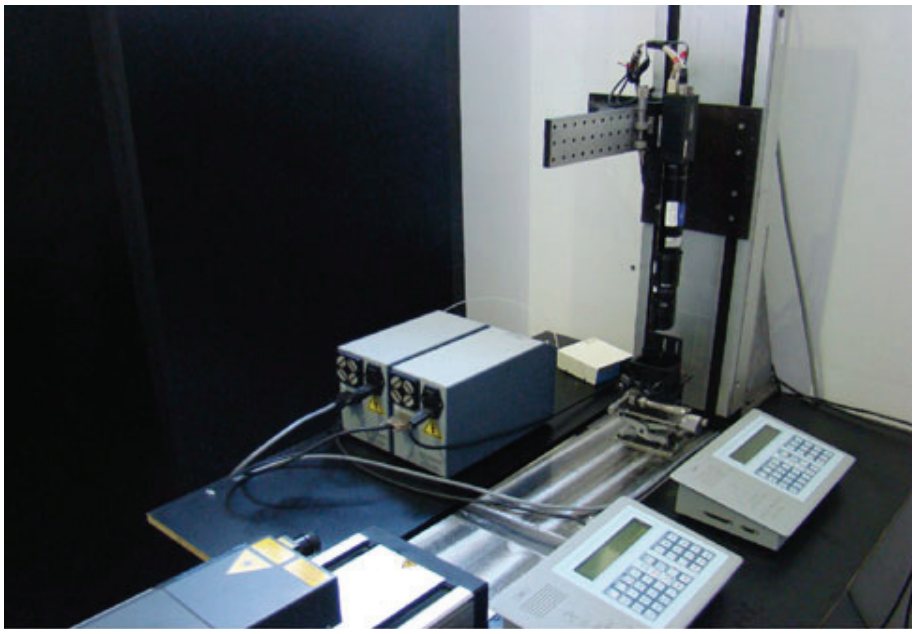


Example of the effect of approach velocity on the coalescence of air bubbles in liquids coalescent ultrapure water and in non-coalescent calcium chloride, c($CaCl_2$) = 0.056 M

Application of the electrodiffusion sensors for the flow diagnostics in microchannels

(J. Tihon, supported by ICPF)

The electrodiffusion technique has been improved to become applicable for the flow measurements in microchannel devices. The technique of photolithography has used to prepare very small but precisely shaped flow sensors. To gain experience with practical measurements on microfluidic scale, the electrodiffusion sensors has been tested under steady flow conditions in straight microchannels. [Ref. 1]

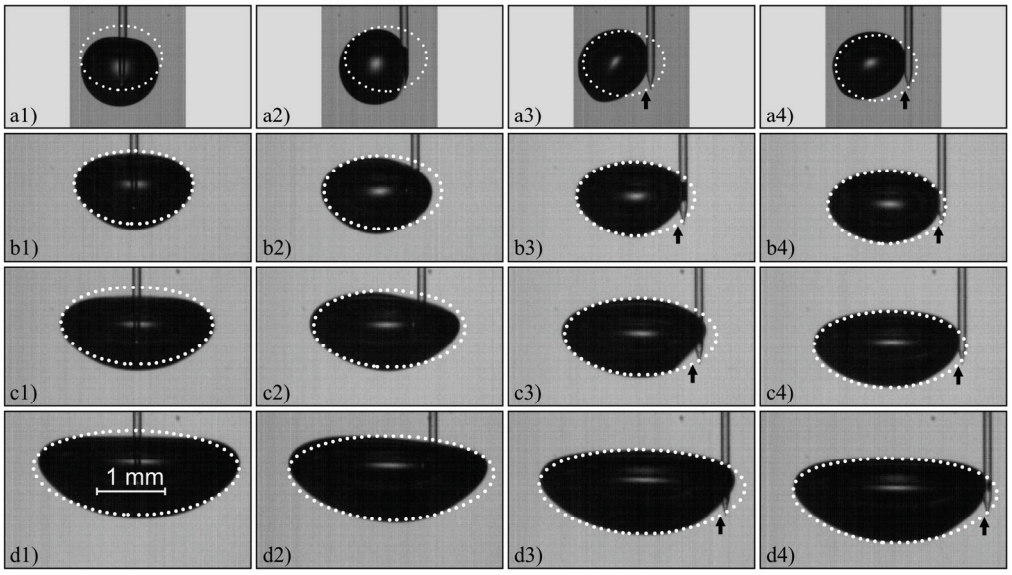


Particle image velocimetry (PIV) set-up

Analysis of hydrodynamic forces acting on bubbles by PIV measurements

(J. Vejražka, supported by ASCR, grant No. IAA200720801)

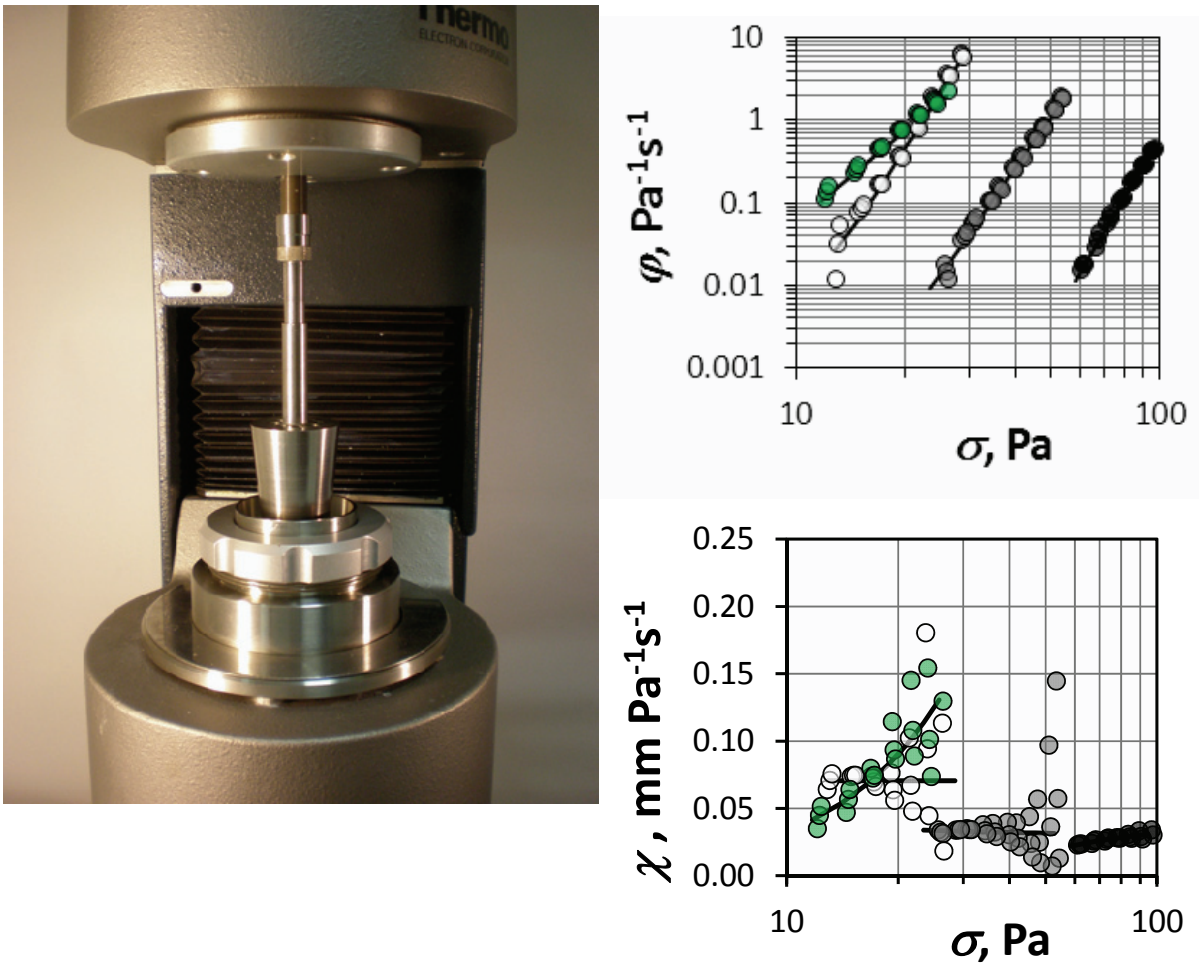
The liquid flow in proximity of bubbles is studied experimentally by using the time-resolved particle image velocimetry and high-speed flow visualizations. The measured velocity field was treated in order to get information on the forces acting on bubbles in different flow situations. The calculation and analysis of the viscous dissipation and inertia of liquid in motion were performed for various situations both in pure liquids and in surfactant solutions. The results were enlarge the knowledge of bubble flow dynamics, required to improve computational models used for the prediction of macroscopic two-phase flows. [Refs. 7, 11, 13, 34, 35, 46-51]



The bubble-probe interaction and comparison of the initial and the terminal bubble shape

Wall effect in flowing microdisperse liquids: apparent slip and electrokinetical potential
(O. Wein, joint project with TU of Ostrava, supported by GACR, grant No. 104/09/0972)

The project aims at a phenomenological characterization of liquid micro-dispersions (aqueous nanofluids and colloidal clay suspensions) by means of three experimental methods. Theory of the electrodiffusion friction probes, including their automated calibration, has been extended to non-linear velocity profiles. AWS viscometry and routine measuring of zeta-potential (ξ) have been applied for a class of nanofluids, prepared using several different dispersing methods. [Refs. 2, 31-33, 43-45]



The AWS (apparent slip at wall) viscometric technique using the novel KK-sensor for microdispersion liquids

Effect of the surface roughness, ohmic resistance, and electrode kinetics on autocalibration of electrodiffusion friction probes
(O. Wein, supported by GACR, grant No. GA104/08/0428)

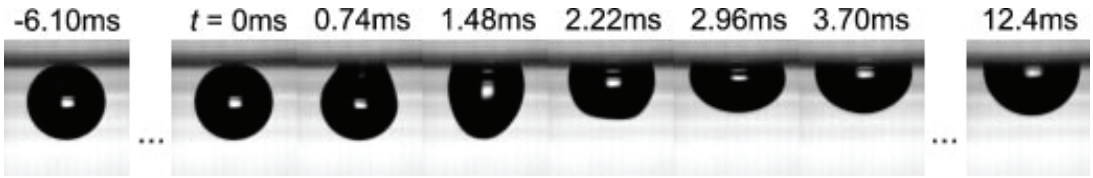
Experimental part of the project consists in studying fast transient processes driven by a step change of voltage in electrolytic microcells. In the first year of the project, an experimental set-up (electrolytic cells, working electrodes, measuring and controlling hardware) were prepared and tested. The programs for PC-driven process control and data acquisition, written under LabView, were prepared and tested. This preparatory activity is documented in a series of three research reports. The related results in electrodiffusion diagnostics of flow were published. [Refs. 6, 8-10, 12, 40-42, 52, 53]

Electrodiffusion friction probes

Hydrodynamics of bubble-particle interactions under liquid circulation

(M. Zedníková, supported by GA ASCR, grant No. KJB200720801)

The project deals with bubble-particle interactions under liquid circulation. Theoretical description exists only for small particle - large bubble interactions, used in mineral flotation. If the objects proportion is inverted, the mechanism of interaction is no longer fully understood. Thus, the objectives of the project are to study: i) small bubble-large particle interactions under liquid circulation and ii) interaction of more bubbles with a particle and formation of stable bubbles-particle aggregate. The bubble trajectory, velocity, momentum and deformation during impact are obtained by high speed camera visualization and the liquid velocity flow field is measured by the particle image velocimetry (PIV). The experimental data were create a base for theoretical description of bubble-particle interactions. [Refs. 11, 17, 25, 56-59]



Sequence of bubble attachment process to the solid surface.
PE surface, deionised water, D_b = 1.05 mm

International co-operations

Berlin Institute of Technology, Germany: Multiphase flow diagnostics
CRTT, Saint Nazaire, France: Microfluidics
Eindhoven University of Technology, the Netherland: Oscillations of fluid particles
Institute of Chemical Engineering, BAS, Sofia, Bulgaria: Gas-liquid reactors
Institute of Fluid Mechanics, Toulouse, France: Effect of surfactants on multiphase flows
Institute of Fluid Mechanics, Toulouse, France: Hydrodynamic interactions of bubbles
Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow
Norwegian Institute of Technology (NTH), SINTEF, Trondheim, Norway: Bubble columns

University of Minho, Braga, Portugal: Multiphase bubble bed reactors
Worchester Polytechnic Institute, Worchester, MA, USA: CFD

Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)
J. Vejražka: IMFT Toulouse, France (1 month)

Visitors

E. Barros, Univiversity of Minho, Portugal (Erasmus)
N. Deshayes, Institut National Polytechnique de Toulouse, France (Intership)
A. Martins, University of Minho, Portugal (Erasmus)
N. Postic, Institut National Polytechnique de Toulouse, France (Intership)
M. Shirota, Hirosaki University, Japan
A. Shirota, Ikadogen Apple Institute Co., Japan

Teaching

J. Drahoš, M. Růžička: ICT, Faculty of Chemical Engineering, postgraduate course "Multiphase Reactors"
J. Havlica: UJEP, Faculty of Science, course "Mathematics for chemists"
J. Tihon, J. Vejražka: ICT, Faculty of Chemical Engineering, postgraduate course "Drops, bubbles, and particles"

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Original papers

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Chapters in books

[15] Gogová Z., Hanika J., Markoš J.: Optimal Design of a Multifunctional Reactor for Catalytic Oxidation of Glucose with Fast Catalyst Deactivation. (Eng) (Brito A.V., Ed.), pp. 209-232, Intech, Vukovar 2010.
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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
- Application of immobilized biocatalysts in optical sensors
- Polymeric antidegradants immobilized on poly(siloxanes)
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphase media
- Carbosilane dendrimers
- NMR spectroscopy

Applied research

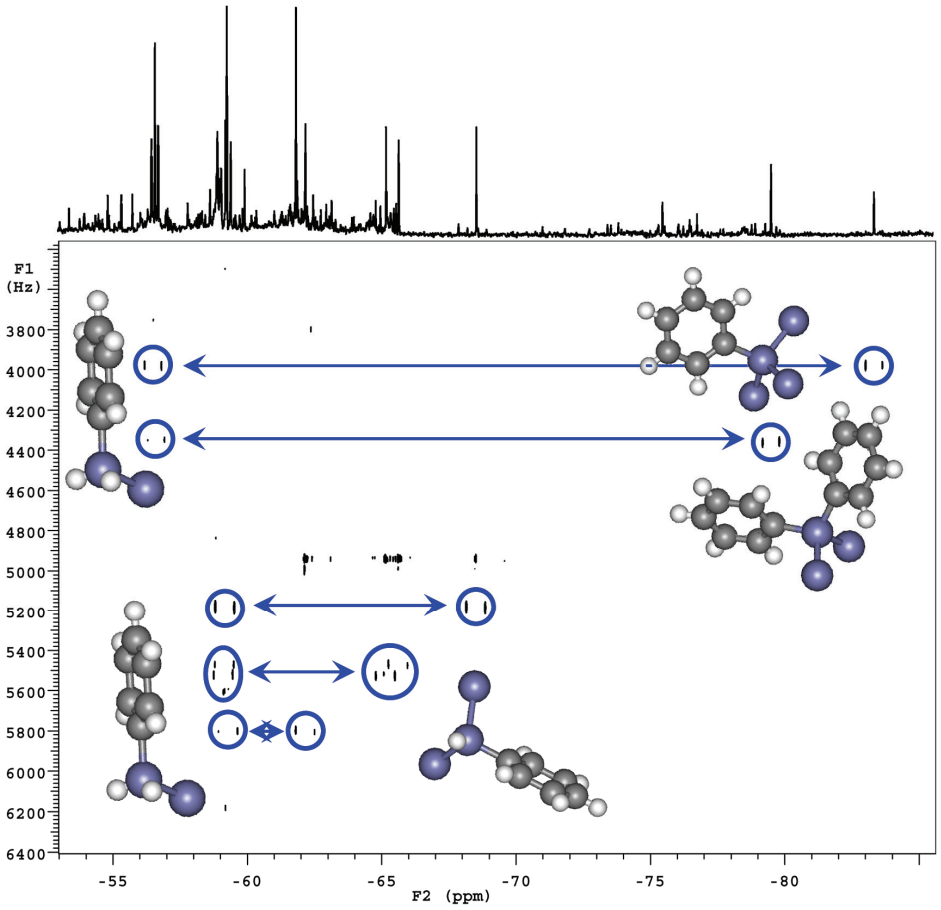
- Complex dehalogenation of PCB contaminated soils, waste water and oils
- Development of new analytical methods
- Analytical services to the research departments of ICPF

Research projects

Dehydrocoupling reactions catalyzed by titanium complexes

(J. Sýkora, joint project with JH IPC, and ICT, supported by GACR, grant No. GA203/09/1574)

Products of dehydrocoupling polymerization reactions were monitored by on-flow LC-NMR and GPC-NMR experiments. Several modifications of the $^{29}Si\{^{1}H\}$ INEPT experiment were implemented to probe the polymer microstructure. The 2D heteronuclear NMR experiments ($^{1}H \rightarrow {}^{29}Si$-$^{29}Si$ INEPT-INADEQUATE and $^{1}H \rightarrow {}^{29}Si$ DOSY) provide valuable information about the branching and length of the oligosilanes. [Refs. 36, 48, 49]

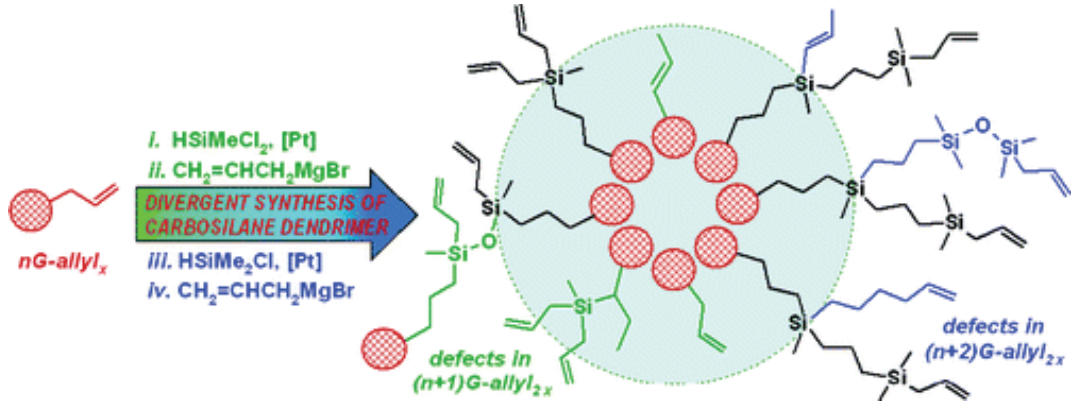


$^{1}H \rightarrow {}^{29}Si$-$^{29}Si$ INEPT-INADEQUATE experiment

The structure and synthetic applications of transition metal complexes

(J. Čermák, joint project with JH IPC, CU, and ICT, supported by MYES, project No. LC06070)

Two ways of immobilization of dichlorotitanocene units to carbosilane dendrimers were studied, the so called inverse and normal hydrosilylations. The normal hydrosilylation, i.e. hydrosilylation of an alkene terminated dendrimer with Si-H-bond-substituted complex gave better results provided that dendrimers were terminated by vinyl instead of allyl terminal groups. Complete analysis of defects in carbosilane dendrimers using combination of MALDI-TOF mass spectrometry and multinuclear NMR spectroscopy was also finished as a knowledge base for future design of dendrimeric structures. Coordination properties of heavy fluorous cyclopentadienes were studied as well. [Refs. 4, 5, 9, 21-25, 32, 47]

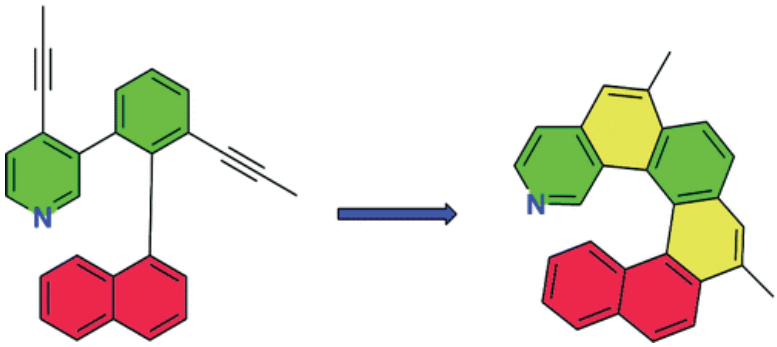


Structural defects in polyallylcarbosilane dendrimers

Synthesis of helicenes via cycloizomerization of biphenylyl-naphthalene and 1,8-diarylnaphthalene derivatives

(J. Čermák, J. Storch, supported by GACR, grant No. P207/10/1124)

The new approach leading to 2-aza[6]helicene was developed being an extension of our previous work published in 2009. It focused on double cycloisomerization of biphenylyl-naphthalene derivatives leading to formation of two aromatic rings in one step. During the last period we have found out a novel tandem cycloisomerization method giving rise to four new aromatic or heteroaromatic rings, yielding various benzo[c]phenanthrene and 6H-naphtho[2,1-c]chromene derivatives. This atom-economic isomerization is now being developed to the synthesis of extended [8]helicene-like molecules. [Refs. 15, 45, 46]

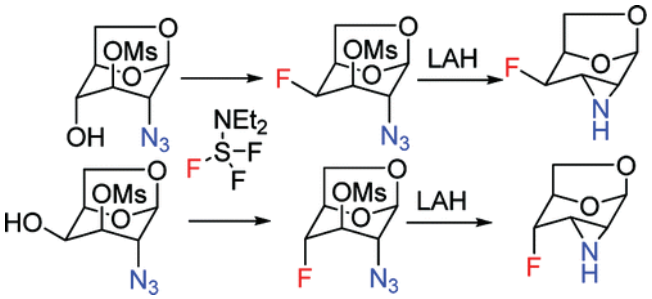


Synthesis of 2-aza[6]helicene utilizing metal-catalyzed cycloisomerization

Reactivity of asymmetrically substituted epimino pyranoses

(J. Karban, joint project with CU, supported by ICPF)

We have finished our work on aziridine-ring cleavage of 4-deoxy-2,3-epimino derivatives of 1,6-anhydro-β-D-hexopyranoses. The regioselectivity of the cleavage was found to be governed by interplay of S_N2 and S_N2-borderline mechanism depending on the type of the nucleophile (hard versus soft) and conditions (acidic versus basic). To further investigate the cleavage mechanism we have prepared the full series of all configurational isomers of 4-fluoro-2,3-epimino-1,6-anhydro-β-D-hexopyranoses. These fluoro compounds were prepared by reaction of suitable azido sulfonates containing a free 4-hydroxyl with diethylaminosulfur trifluoride and subsequent reductive cyclization. The study of their reactivity is now in progress. [Refs. 7, 12, 13, 16, 30, 31, 37, 42, 43, 51]

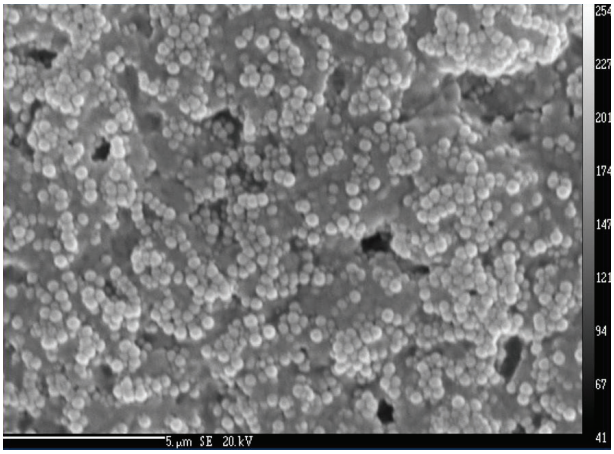


Synthesis of 1,6-anhydro-2,3,4-trideoxy-4-fluoro-2,3-epimino-β-D-hexopyranoses

Monitoring and remediation of environmental pollution with advanced organic-inorganic materials – MOREPIM

(G. Kuncová, supported by MEYS, KONTAKT project No. ME 892)

The research has been focused on utilization of inorganic and organic-inorganic nanoparticles in design of optical fibre sensors for monitoring of environmental pollution [Ref. 11, 17, 29, 34, 52].

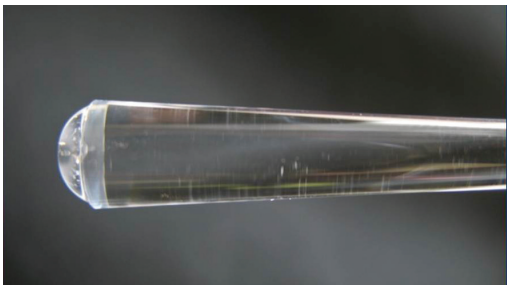


Fixation of bioluminescent biorepoters with silica nanoparticles

Whole cell optical sensors (WOCOS)

(G. Kuncová, supported by MEYS, KONTAKT project No. ME 893)

Bioluminescent bioreporters were immobilized on front faces of optical fibres with aim to prepare optical fibre sensors for in situ monitoring in remote localities. We calculated that only 3.5% of all photons, produced by one bacterium placed on the front end of the optical fibre are coupled and guided. Up to six times higher intensity of detected light was calculated and measured by enlargement of an area covered with bacteria using the front face of optical fibre with appropriate shape. [Refs. 2, 33, 40, 52]

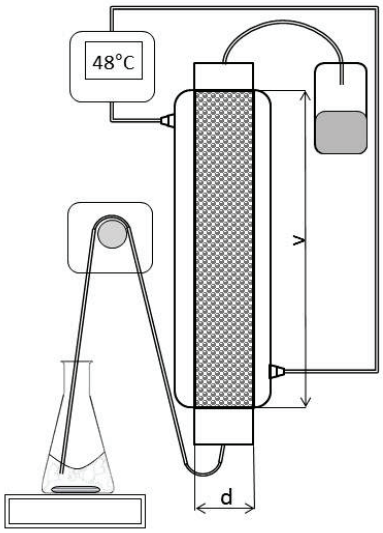


The tip of tappered quartz optical fibre (Ø=10 mm) coated with *Pseudomonas putida* TVA8 encapsulated in silica gel

Enzymatically catalyzed synthesis of alkyd resins (ENZALKYD)

(G. Kuncová, joint project with SYNPO Pardubice a.s., supported by MIT, project No. MPO 2A-3TP1/108)

The research has been focused on continuous glycerolysis of soybean oil catalyzed with immobilized enzyme in column reactor. [Refs. 19, 20]

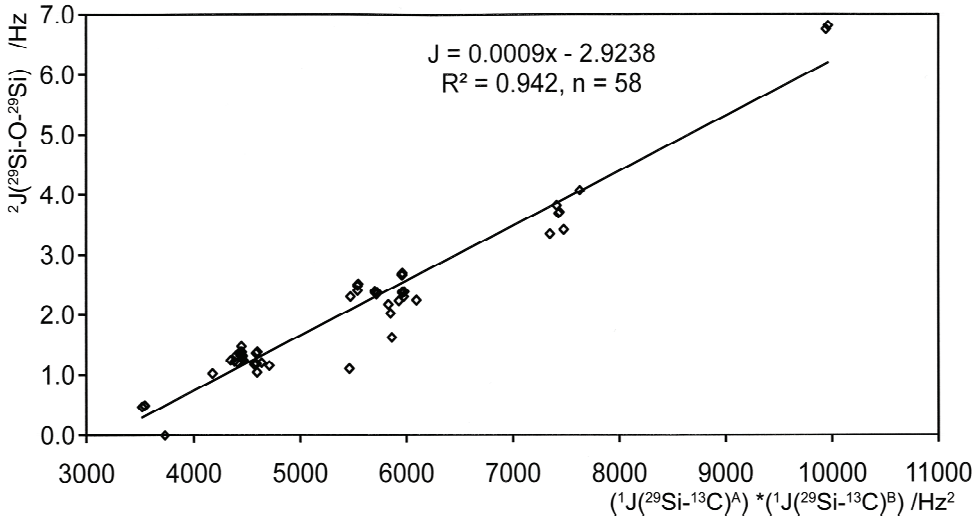


Column reactor for continuous glycerolysis of vegetable oils catalyzed with immobilized lipase

^{29}Si-NMR structural analysis of branched organosilicon polymers and its application in LC-NMR

(J. Kurfürst, supported by GACR, grant No. GP203/08/P412)

^{29}Si-O-^{29}Si coupling constants were determined for a series of 56 siloxanes and empirical correlations were found between these couplings and number of oxygen atoms attached or the sum of ^{29}Si chemical shift. The correlation with the product of $^{1}J(^{29}Si\text{-}^{13}C)$ couplings was put on a theoretical basis. [Ref. 3]

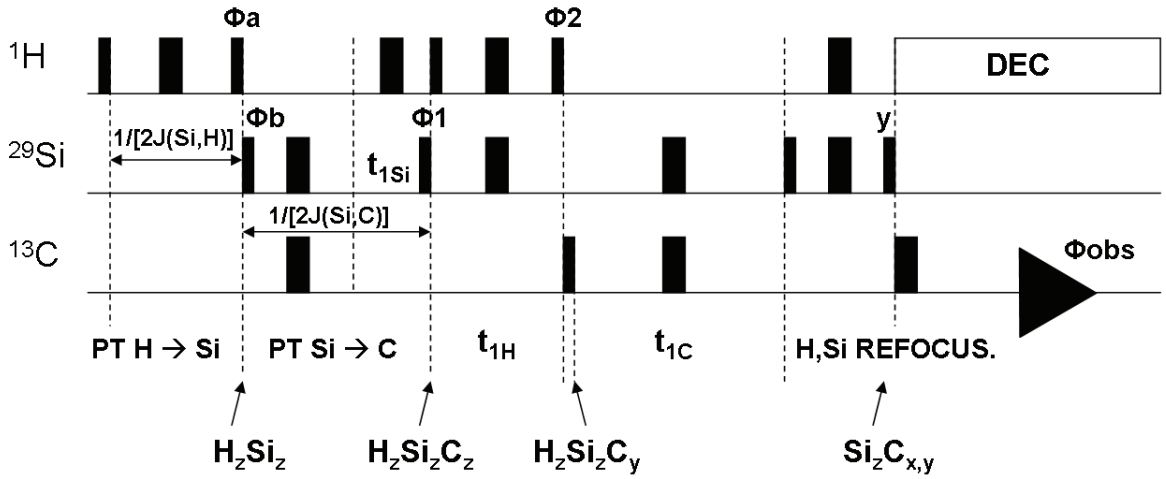


Correlation between geminal two-bond coupling $^{2}J(^{29}Si\text{-}O\text{-}^{29}Si)$ and one-bond couplings $^{1}J(^{29}Si\text{-}^{13}C)$ in methylsiloxanes

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

(J. Schraml, supported by ASCR, grant No. IAA400720706)

New methods for measurement of signs of spin-spin couplings between ^{29}Si and ^{13}C or ^{1}H nuclei in solutions utilize instrumental possibilities of triple resonance of ^{1}H-^{13}C-^{29}Si nuclei. Using these experiments model series of compounds have been measured [Refs. 1, 10, 18, 44].

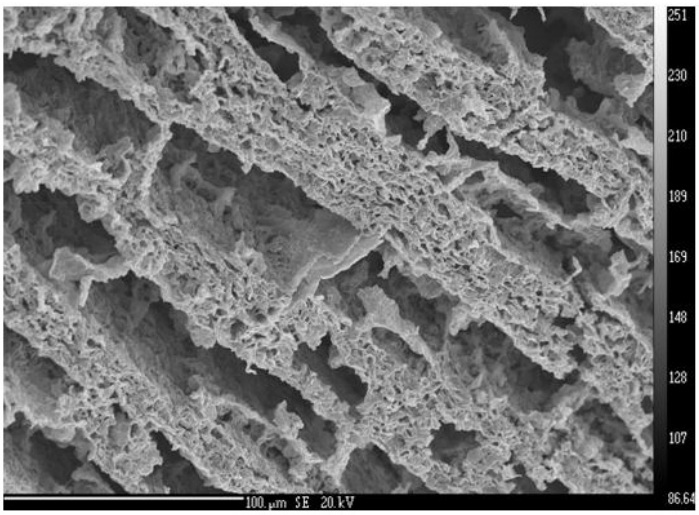


NMR Pulse sequence for determination of the signs of heteronuclear coupling constants

Novel inorganic-organic hybrid nanomaterials

(S. Šabata, joint project with ICT Prague, IMC, University of West Bohemia Plzeň, supported by ASCR, grant No. IAAX08240901)

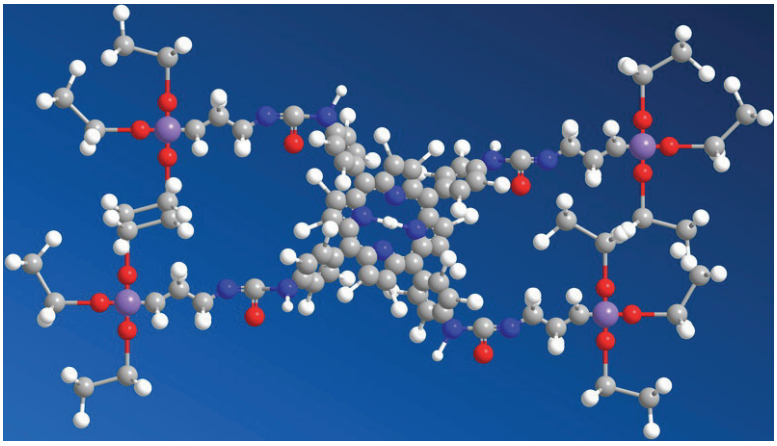
Na^+ montmorillonite was silanized with methoxy- and ethoxy- organosilanes having functional groups; $-C_3H_7NH_2$, $-CH_2CH{=}CH_2$, $-C_8H_{17}$, $-C_{18}H_{37}$, $-C_3H_7C{\equiv}N$. The products were characterized with X-Ray. Enzyme lipase was adsorbed on modified montmorillonites. The highest catalytic activity, in esterification of steraic acid with propanol, performed biocatalyst prepared by adsorption of Lipolase 100L on montmorillonite with $-C_{18}H_{37}$.[Ref. 6, 8, 26-28, 33, 50]



The SEM micrographs of cross sections of lipase catalyst (cloisite modified with octadecyltrimethoxysilane) formed by ice-templating processes

Calixarene-porphyrin conjugates for selective complexation and separation of fullerenes
(S. Šabata, joint project with ICT, IIC, supported by GACR, grant No. 203/09/0691)

Novel technique of silanization of aminoporphyrines and thiacalixarenes was developed. The silanization products of tetraaminoporphyrine and thiacalixarene were characterized with ^{1}H-NMR and ^{13}C-NMR spectroscopy. Silanized tetraaminoporphyrine was immobilized on silica carrier and this material has been tested as filling of HPLC column. [Ref. 50]



Silanized tetraaminoporphyrine

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

Instituto Supérior Técnico, Lisbon, Portugal: Chemistry of transition metal complexes with azine ligands

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

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Chapters in books

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International conferences

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Environmental Process Engineering Laboratory

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Fields of research

- Persistent organic pollutants
- Fluidized bed combustion and gasification
- Gas-solid reactors and operations
- Gaseous and particulate emissions from combustion and industrial processes
- Preparation of the electrodeless discharge lamps for photochemical applications
- Electrodeless discharge lamps coated with the titania-doped thin films for photocatalysis in the microwave field
- Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis

Applied research

- Recovery of precious metals
- Electronic scrap recycling
- Phytoextraction biomass disposal
- Simultaneous disinfection and microwave drying of materials
- Technology of repairing roads with asphalt material
- Microwave method and device for recycling refined steel cord from waste tires
- Low-energy microwave depolymerization of wastes poly(ethylene terephthalate) (PET) and polyurethane (PUR) foam

Research projects

Near zero emission advanced fluidized bed gasification (FLEXGAS)

(M. Punčochář, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00005)

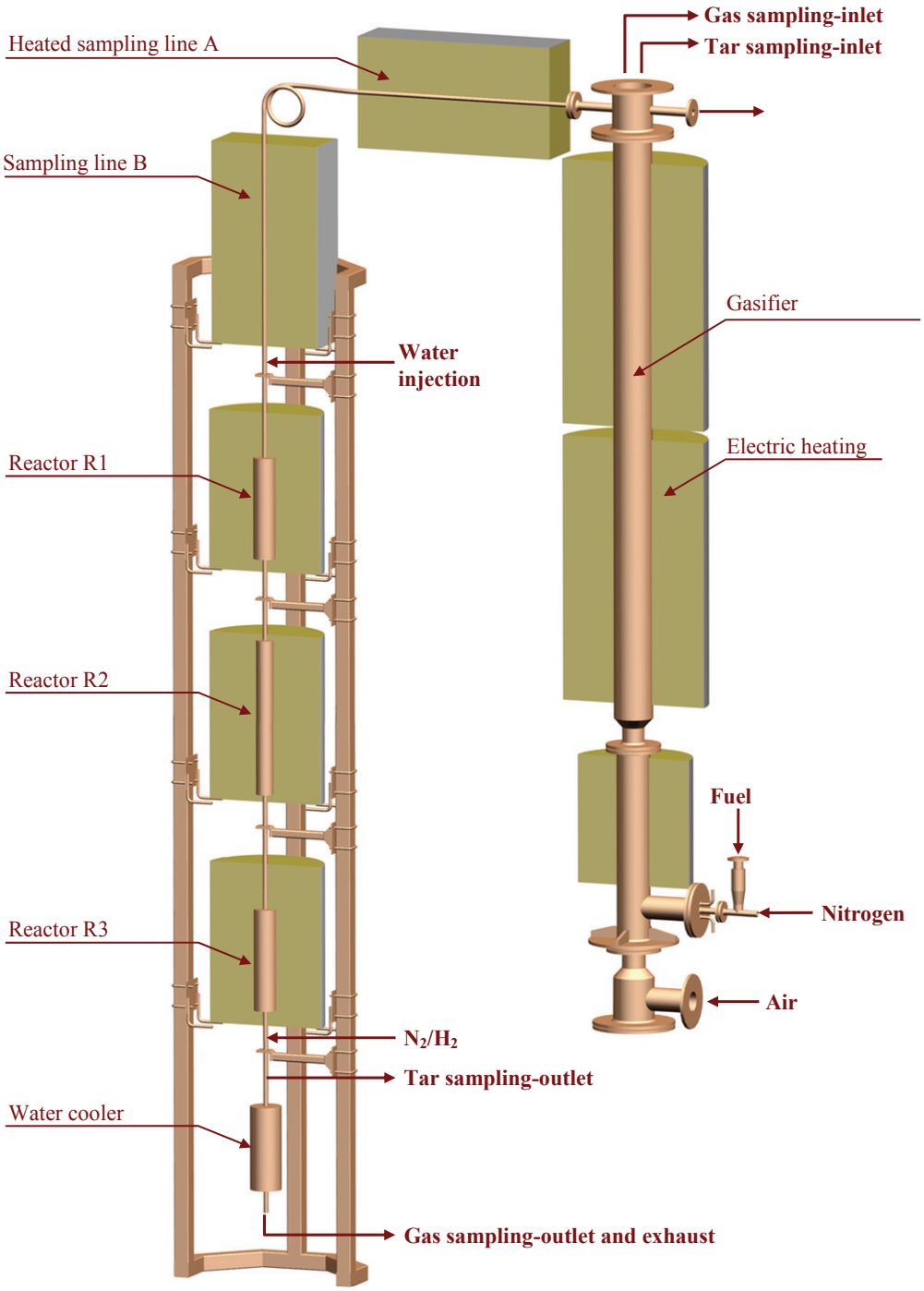
Ways of overcoming the potential disadvantages of fluidized bed gasification, the technology for CO_2 capture/reduction and the advantages in terms of their ability to process biomass/waste in association with coal at different scales of operation and for different applications were examined. [Refs. 6, 18, 37, 44 -48]

Fluidized bed gasifier

Waste as raw material and energy source (WARMES)

(M. Punčochář, joint project with Brno University of Technology, and EVECO Brno s.r.o., supported by MEYS, project No. 2B08048)

The project is concerned with research and application of modern approaches leading to the higher efficiency in using different classes of wastes in energy and recycling processes. Attention is paid especially to the processes of thermal processing of wastes with the aim of maximal use of produced energy with minimization of released harmful substances. Project involves both experiments and computer simulations. [Refs. 8, 19, 20, 23, 41, 42, 52, 53]

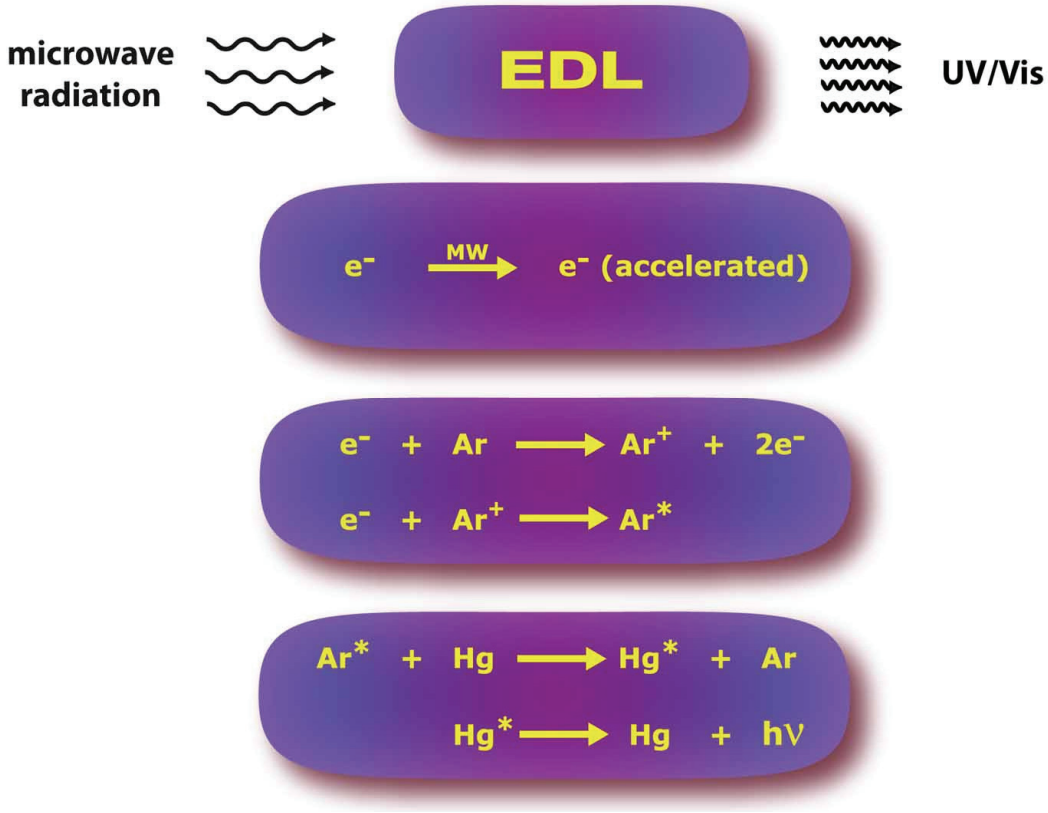


Gasifier and gas cleaning unit

Preparation of the electrodeless discharge lamps for photochemical applications

(V. Církva, supported by ICPF)

The project is concerning on preparation of the electrodeless discharge lamps (EDLs) as a suitable source of UV/Vis light for photochemical reactions. The EDL consisted of a glass tube filled under a lower pressure with an inert gas and an excitable substance (mercury, sulfur), and generated UV/Vis radiation when placed into the microwave field. The effect of operating EDL parameters, the microwave power output and medium properties on spectral characteristics has been studied. [Refs. 1, 7, 21, 22]

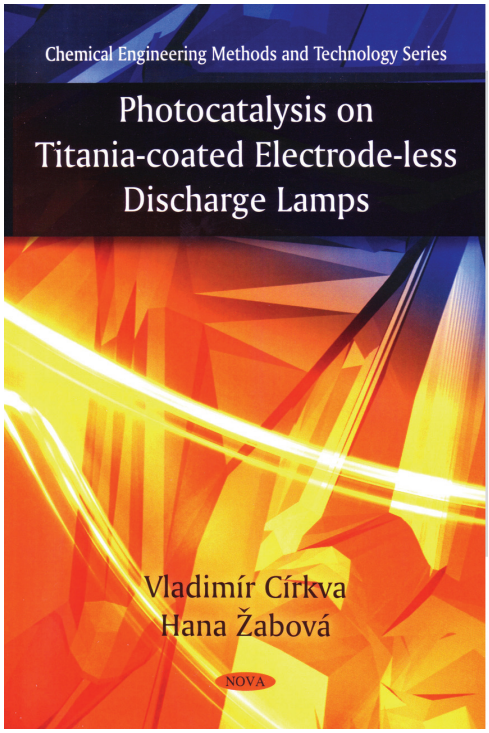


Principle of Hg-EDL operation and the release of emission energy as UV/Vis radiation

Electrodeless discharge lamps coated with the titania-doped thin films for photocatalysis in the microwave field

(V. Církva, supported by ICPF)

Research has been aimed to prepare a visible-light response photocatalyst in the form of thin film on the electrodeless discharge lamps (EDLs). Titanium dioxide nanoparticles were also doped with various ions of transition metals M (i.e. M = Fe, Cr, Mn, Co, V, Zr, Ni, Ag). Thin films of titania were prepared by using the sol-gel methods (titanium isopropoxide, titanium *n*-butoxide, acetylacetone, and a transition metal acetylacetonate) and dip-coating technique. The films were characterized through XRD, Raman spectroscopy, XPS, SEM, AFM, and UV/Vis. Photocatalytic activity of the prepared titania-doped thin films has been evaluated by the decomposition of Rhodamine B in water and on degradation of aqueous solution of mono-chloroacetic acid (0.1 mol l^{-1}) in a microwave field using the coated EDLs. Also the effect of operational parameters was reported for both batch photoreactor (number of coating cycles for EDL, light intensity, initial pH value, and H_2O_2 dosage) and for continuous-flow set-up (flow rate, number of titania-coated EDLs, reaction temperature, and air bubbling). [Refs. 5, 17, 21, 22]



Photocatalysis on Titania-coated EDLs (book), the modified MW oven, and coated Hg-EDL

New technologies for recovery of rare and special metals from electrical and electrotechnical wastes

(V. Gruber, joint project with SAFINA a.s., supported by MIT, IMPULS project No. FI-IMS/075)

The project deals with recovery of rare metals from electrical and electrotechnical wastes. Special attention is paid to the recovery of Eu and Y from TV sets. [Refs. 24, 33]

Apparatus for recovery of rare metals

Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis

(M. Hájek, supported by GACR, grant No. GA104/08/0416)

The research has been focused on application in heterogeneously catalyzed reactions in liquid phase. It has been observed that selectivity of catalytic reaction can be significantly improved. These important findings evoked continuation to study this effect in more detail, what is the subject of this project. Scope and limitation of this method including possibility of potential applications has been studied on model reactions with non-polar (non-absorbing) reactants (alkylation of aromatics by cycloalkenes) in the presence of strong acidic (strong absorbing) solid catalysts. [Refs. 4, 15, 16, 38–40, 43]

Simultaneous disinfection and microwave drying of books and similar paper-based materials

(M. Hájek, supported by ICPF)

An advanced microwave drying technology has been developed using a microwave continuous dryer combined with an air cooling unit and a simultaneous disinfection process. This new technology uses microwave absorption filters made from special porous ceramics which act as both absorbent and transparent material for microwaves. Ceramic slabs reduce the intensity of the microwave radiation to such an extent that overheating and hot-spot formation as well as red-heating of metallic objects and other kinds of damage is prevented. [Refs. 2, 34]

Continuous microwave drying equipment

Device for repairing roads with asphalt material

(M. Hájek, supported by ICPF)

The device and method of microwave heating has been applied for repairing roads with asphalt material. [Refs. 25, 29]

Microwave method and device for recycling refined steel cord from waste tires

(M. Hájek, supported by ICPF)

This method was used for refining metal material separated from crushed waste tires by microwave heating the metal material (comprising steel cord containing 82-98 % of steel by weight) and distilling off a portion of non-metallic constituents. [Refs. 26, 28, 56, 57]

Low-energy microwave depolymerization of waste poly(ethylene terephthalate) (PET) and polyurethane (PUR) foam

(M. Hájek, supported by ICPF)

Microwave energy has been applied for total depolymerization of waste PET material, especially waste PET bottles. The products were terephthalic acid and ethylene glycol. The process included the following steps: depolymerization, purification and separation. Total depolymerization was achieved by applying microwave energy of 2450 MHz frequency with energy consumption of 0.5 - 1.0 kWh/kg PET. A developed recycling process has been based on the chemolysis of polyurethane (PUR) foam using proper diols or triols in combination with microwaves heating. The product was a liquid recyclate with active hydroxyl groups. [Refs. 27, 30, 31]

Purified terephthalic acid

Fluidization and decontamination of organic-polluted solids in a fluid-bed reactor

(M. Hartman, supported by ASCR, grant No. IAA400720701)

A fundamental understanding of such viable reaction systems for the thermal oxidation of organic liquids entrapped (absorbed) within porous solids is still lacking. The hydrodynamic behaviour of the "g"-"s" suspensions with such polluted (wet and sticky) particles is explored with the aid of pressure fluctuations also with respect to their unwanted tendency to stick together and lie down. Hitherto unexplored, inert and porous particles

soaked in model organic compounds will be fired in a bench-scale, fluid-bed reactor operated in different regimes. Experimental and modelling efforts seek to explain and describe the dependence of the reactor's combustion efficiency as a function of residence time, excess air, operating temperature and particle size. The study focuses on the overall picture of formation and oxidation destruction of main gaseous pollutants (NO, NO_2, N_2O, CO, organic residuals, persistent organic pollutants, SO_2, and HCl) and their interrelationships. [Refs. 3, 12, 13]

Fluidized bed reactor

Immobilization of heavy metals in municipal waste incinerator materials

(M. Šyc, supported by European Economic Area (EEA) and Norway grant intermediate by the National Training Fund, project A/CZ0046/1/0027)

The combustion of municipal waste is one of ways to meet nowadays the EU requirements to reduction of amount of dumped waste. The municipal solid waste incinerators (MSWI) convert waste to energy and certain amount of solid waste materials – fly ash and bottom ash. These solid residuals contain, besides other components, toxic heavy metals which have to be stabilized against leaching out from the waste material before it can be safely stored at a land-fill. The MSWI solid waste materials have latent hydraulic or puzzled

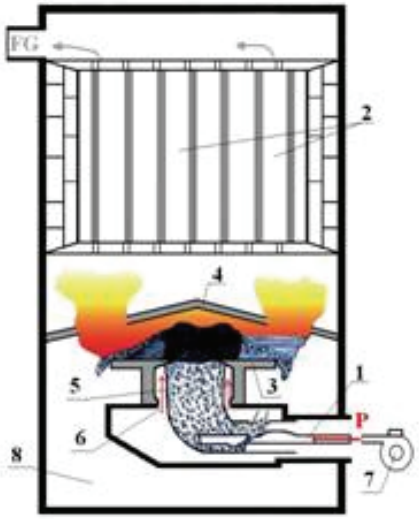
properties. This fact offers an effective way of heavy metals immobilization which is studied in the present project. [Refs. 9, 19, 50, 51]

Samples of concrete immobilizates

Emission factors of POPs and heavy metals from small sources

(M. Šyc, V. Pekárek, joint project with TU of Ostrava, supported by MEYS, project No. SP/1a2/116/07)

Determination of emission factor for selected POPs compounds and heavy metals is solved. The following topics were studied (i) the validation of the original air dilution unit for the sampling, (ii) effect of different combustion units from the standpoint of toxic compound emission, and (iii) effect of different fuels on the toxic compounds formation. [Refs. 11, 49]

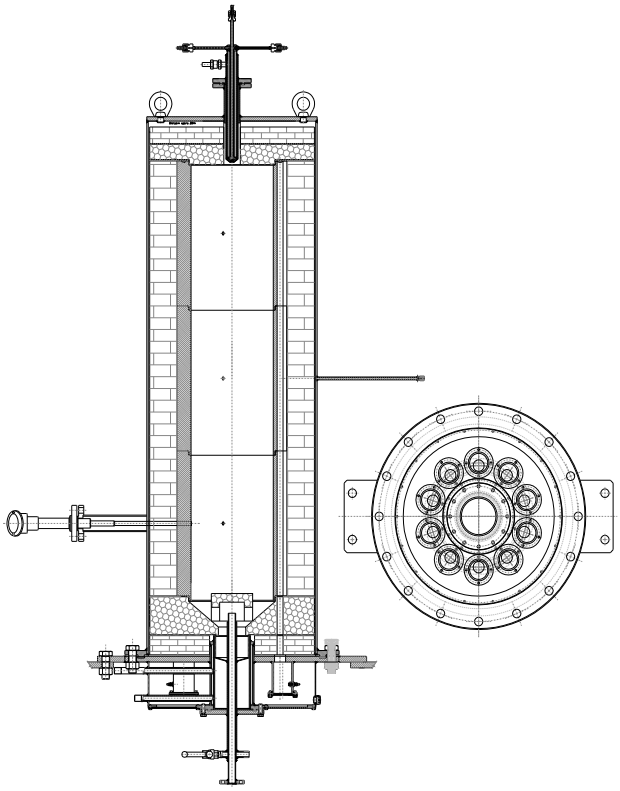


Scheme of automatic under-fire boiler with screw conveyor

Research of hydrogen and synthesis gas production by gasification of waste biomass originating from the production of biofuels

(V. Veselý, J. Hanika, joint project with Research Institute of Inorganic Chemistry, Ústí n/L, supported by MIT, project No. 2A-2TP1/024)

Project is focused on gasification of waste biomass which comes from the production of bio-ethanol and bio-diesel. The aim is to produce hydrogen from biomass, to capture CO_2 rising in the process and to separate present heteroatoms. A specific task of the project is to develop the integral process which includes the processing of biomass into existing technology of crude oil waste gasification. [Refs. 10, 14, 32, 35, 36, 54, 55]



Pilot plant gasification reactor

International co-operations

Central Mechanical Engineering Research Institute, Durgapur, India: Gasification
Institute for Energy, Joint Research Centre, Petten, the Netherlands: Pressurized fluidized bed combustion/gasification technologies; Waste incineration/gasification
University of KwaZulu-Natal, Durban, Republic of South Africa: Gaseous and particulate emissions
Vienna University of Technology, Vienna, Austria: Gasification

Teaching

V. Církva: ICT, Faculty of Chemical Technology, postgraduate course "Microwave Chemistry"
V. Církva: ICT, Faculty of Chemical Technology, postgraduate course "Photochemistry"
M. Punčochář: Czech University of Life Sciences Prague, course "Renewable and alternative sources of energy"
K. Svoboda: UJEP, Faculty of Environment, courses "Decontamination and Bio-remediation Technologies" and "Energetics (Power generation) and Protection of the Environment"

Publications

Original papers

[1] Církva V., Relich S., Hájek M.: Microwave Photochemistry V: Low-Pressure Batch and Continuous-Flow Microwave Photoreactors with Quartz Mercury Electrodeless Discharge Lamps. Photohydrolysis of Mono-Chloroacetic Acid. (Eng) J. Chem. Technol. Biotechnol. 85(2), 185-191 (2010).

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Fields of research

- Composition, size and hygroscopicity of 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
- Combustion aerosols
- Emissions sampling
- IR and UV laser induced chemistry
- Chemical vapour deposition of novel Si- , Ge- and C-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

Research projects

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

(V. Ždímal, joint project with CTU and Institute of Thermomechanics of the ASCR, v. v. i., supported by GACR, grant No. GA101/09/1633)

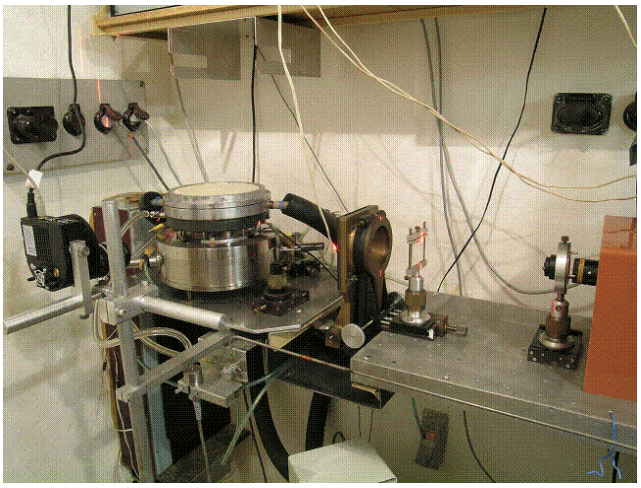
The aim of the project is to determine some properties of heterogeneous nuclei present in the superheated steam of steam turbines. In this project, the sampling device, coupled to advanced aerosol instrumentation (condensation particle counter, scanning mobility particle sizer), was used to measure heterogeneous particles at selected power stations. To enable measurements of particles down to about 1 nm, a fast expansion chamber was developed, enabling resolution of particle size by variable supersaturation. Collected data are served 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. 17-19, 51, 59, 60, 62-64, 66, 92]

Aerosol sampling train connected to the turbine at thermal power plant Prunéřov II

Thermophysical properties of water in unexplored, technologically significant regions

(V. Ždímal, joint project with Institute of Thermomechanics of the ASCR, v. v. i., CTU, and University of West Bohemia, Plzeň, supported by ASCR, grant No. IAA4200760905)

This project was focused 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 are providing first data. A new method and apparatus have been developed. The surface tension of supercooled water and a salt solution was measured. The surface tension of nano-droplets was estimated from nucleation experiments. A range of theoretical approaches including phenomenological methods, simplified microscopic models, and molecular simulations, has been used with experimental data to obtain fundamental findings and engineering models. [Refs. 2, 3, 17, 19, 59, 60, 64, 65]



Thermal diffusion cloud chamber built at the ICPF - on the optical bench

New ways to synthesize nanoparticles of various oxides

(V. Ždímal, joint project with the ICT and Spolchemie a.s., supported by the MIT-FR, grant No. FR-TI1/548, 2009-2012)

The aim of the project is to seek new ways how to synthesize nanoparticles of various oxides, characterize produced particles and perform a process scale–up. [Refs. 18, 56, 61, 84]

Electrostatic classifier built at the ICPF for separation of aerosol nanoparticles

European supersites for atmospheric aerosol research (EUSAAR)

(J. Schwarz, supported by European Commission, project No. FP6-026140-EUSAAR)

European infrastructure project EUSAAR is focused on improving the current state of aerosol measurement on European supersites for atmospheric aerosol measurement. This aim is being reached by dissemination of knowledge from basic technical level to setting-up a state of the art of experimental methods on selected sites. QA/QC procedures, intercalibration

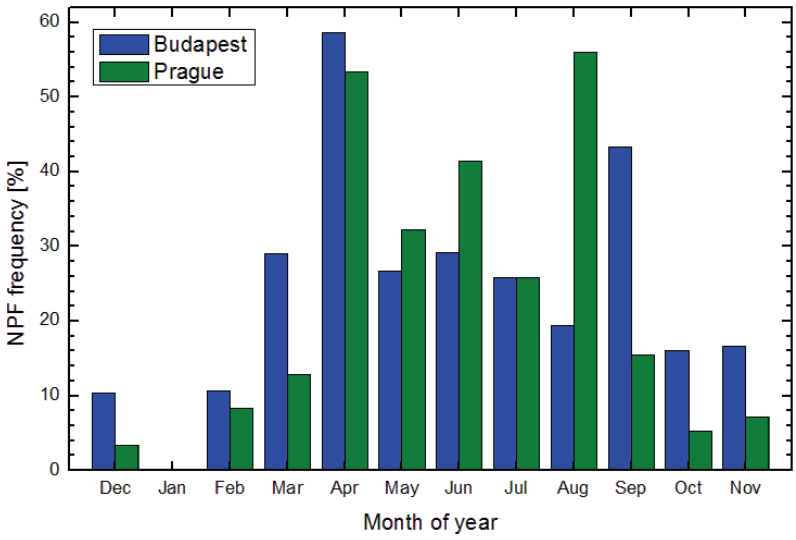
of both basic and advanced measurement methods together with development of new aerosol instrumentation are the ways to fulfill the aims of the project. [Refs. 77, 88, 90, 91]

Košetice supersite (OBK) as a part of European supersites for atmospheric aerosol research

Similarities and differences of ultrafine urban aerosol in Budapest and Prague

(J. Schwarz, supported by MEYS, KONTAKT Mobility project No. MEB 040916)

The main objectives of the project are to determine the concentrations, size distributions and other relevant properties of the ultrafine aerosol particles in Budapest and Prague, to intercompare the measuring results and conclusions for both capitals in order to identify general properties and specialities, to assess the relationships between the size distribution and deposition in the human respiratory system for the ultrafine aerosol, and to study the dynamics of the new aerosol particle formation and growth including specialities in Budapest and Prague.

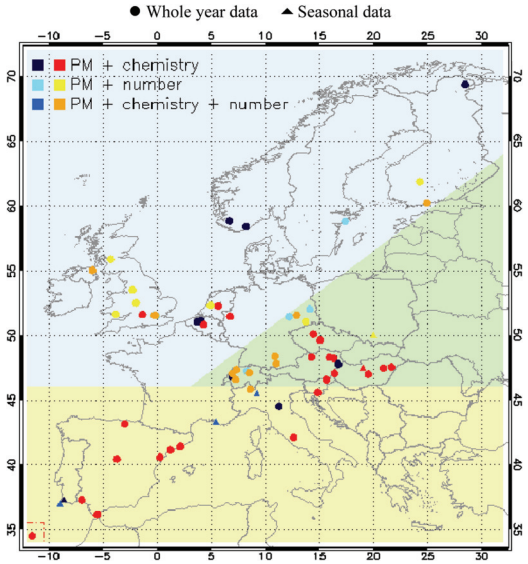


Nucleation frequency during one-year measurement period in Prague and Budapest

Comparison of aerosol composition, source region profiles and types observed in 1994 and 2009 at rural background site in Central Europe

(J. Schwarz, joint project with Nuclear Physics Institute of the ASCR, v. v. i., supported by GACR, grant No. GA205/09/2055)

The objectives of project can be summarized as follows: Atmospheric aerosol elemental composition on daily based samples are analyzed using high sensitive non-destructive multi-elemental analytical technique (Proton Induced X-ray Emission PIXE), using multivariate statistical methods the main aerosol source types and their elemental profiles as well as magnitude of their influence on receptor site are identified. Main source regions and their impact on regional air quality are studied by combining the aerosol composition analysis with air mass transport history study. The obtained results are compared with data available from 1990s to assess the impact of economical and structural changes in Central European economy on air pollution. [Refs. 31, 36, 74, 79, 86, 87]

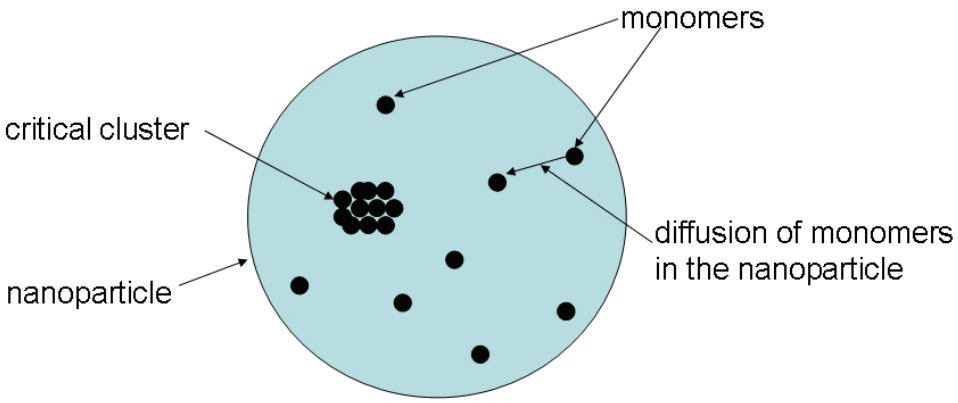


Location of the sampling sites. The pastel background colours delimit the 3 geographical sectors Northwestern, Southern, and Central Europe

Influence of surface processes and electromagnetic radiation on transfer phenomena in aerosol systems with nanoparticles and porous bodies with nanopores

(V.V. Levdanski, supported by ASCR, grant No. IAA400720804)

Aims of the project is to perform a theoretical study of the influence of surface processes, size effects and electromagnetic radiation on transfer phenomena in aerosol systems with nanoparticles and in capillary-porous bodies with nanoscale pores taking into account physicochemical transformations on the particle and pore surface. Study of the joint influence of size effects, electric charge and adsorbable foreign gases on formation of nanoparticles was made as well. Novel methods of the membrane purification of gases under influence of resonance radiation were considered. The effect of radiation on mass transfer and storage of hydrogen in metallic nanoparticles was investigated. The influence of electromagnetic radiation on coagulation, coalescence of nanoparticles and their deposition on a surface has been observed. [Refs. 16-19, 59-66]

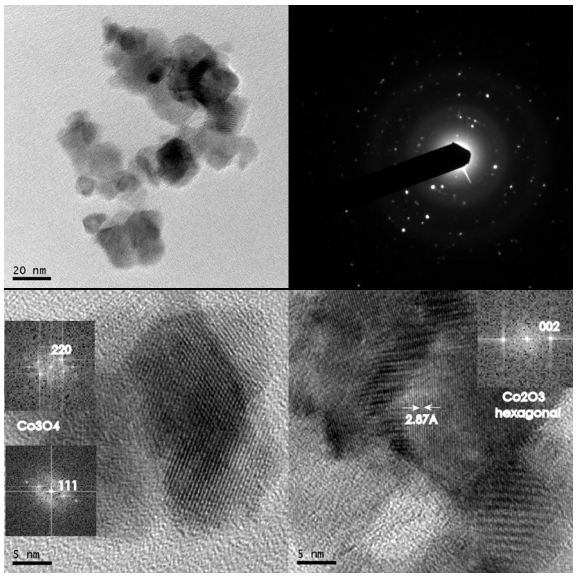


The size dependence of nucleation rate

Composite nanoparticle synthesis by an aerosol process

(P. Moravec, joint project with IIC, and Tampere University of Technology, Finland, supported by GACR, grant No. GA104/07/1093)

Project involves an experimental study of nanoparticle synthesis by chemical vapour condensation method in an externally heated tube flow reactor. In the first part of the project: (i) single component metal and ceramic particles (Co, Ni, Pd, MnO) with great potential of applications are prepared by thermal decomposition of corresponding metal-organic compounds. In the next step: (ii) binary mixed or coated metal-ceramic particles (TiO_2-Co, Al_2O_3-Ni, Al_2O_3-Pd) with potential use as catalyst and binary metal-ceramic (Co-SiO_2) and ceramic-ceramic (MnO-SiO_2) particles with potential applications as gas sensors or in electronics are prepared by simultaneous decomposition of two precursors. Particle morphology, crystallinity, and chemical composition were examined by SEM, TEM, SAED, XRD, EDS, etc. Results obtained in a hot wall reactor have been compared with those from experiments with liquid flame spray reactor at Tampere University of Technology. [Refs. 15, 23, 58, 61-63, 66, 71, 72]

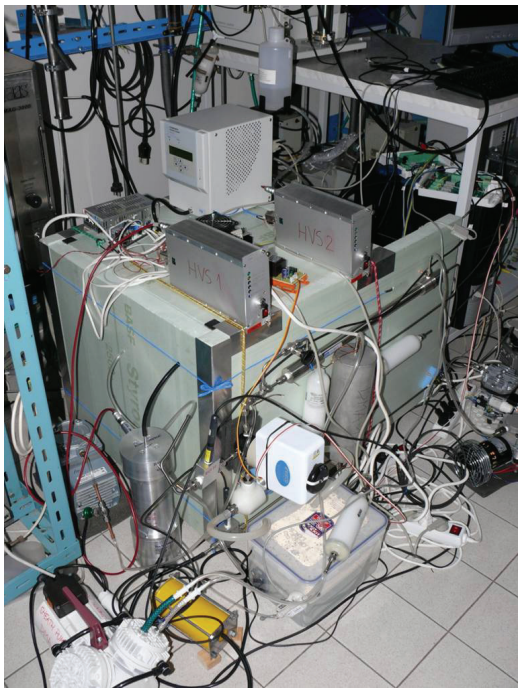


HRTEM images and SAED pattern of CoO_x nanoparticles synthesized by oxidation of CoAA

European integrated project on aerosol cloud climate and air quality interactions (EUCAARI)

(J. Smolík, supported by EC, project No. FP6-036833-2-EUCAARI)

European infrastructure project EUCAARI is designed as a research chain that aims to advance our understanding of climate and air quality through a series of connected activities beginning at the molecular scale and finishing at the regional and global scale. EUCAARI is build upon the pool of available data from previous field campaigns and long-term measurements in order to establish globally consistent data sets. A hierarchy of complementary models, at the molecular, process, meso-, regional and global scales has been applied in a coordinated way in EUCAARI. [Refs. 11, 12, 78, 89]



Hygroscopic Tandem Differential Mobility Analyzer (HTDMA) for measurements of hygroscopic properties of atmospheric aerosol particles

Improvement of the assessment methods of ambient air pollution loads of PM10 in the Czech Republic

(J. Smolík, joint project with Czech Hydrometeorological Institute, and Norwegian Institute for Air Research, supported by Norwegian Funds (via Ministry of Finance of the CR), project No. CZ 0049)

The aim of the project is to improve the characterization of PM10 suspended particles with the focus on secondary particle contribution, proposal of chemical model of secondary particles formation, identification of sources, and application and verification of dispersion models. The project provides direct support to the improvement of ambient air quality in the Czech Republic, respects the principle of air pollution prevention and meets the conception of sustainable development. [Refs. 2, 4, 8, 9, 10, 21, 35, 41, 42, 52, 69]

Determination of chemical and toxicological properties of suspended particles and study of their formation

(J. Smolík, joint project with Czech Hydrometeorological Institute, Technical Services for Air Protection, Institute of Analytical Chemistry of the ASCR, National Institute of Public Health, and TU of Ostrava, supported by Ministry of Environment, grant No. SP/1A3/148/08)

The aim of the proposed project is to suggest possible legal measures to decrease level of atmospheric aerosol burden in the Czech Republic. The sampling and chemical analysis of both particulate emissions and immissions at several types of sources and places in the Czech Republic, statistical analysis of the results and toxicological characterization of particles have been used to fulfill the aim of the project. [Ref. 34, 47-50, 53, 55, 73, 78, 80]

Chemical interactions between cultural artefacts and indoor environment (EnviArt)

(J. Smolík, supported by European Science Foundation (ESF), COST Action D42)

The aim of EnviArt is to explore chemical interactions between cultural artefacts and typical indoor environmental conditions through field studies and laboratory experiments and transfer the results into preventive conservation practice. The Action focuses on the chemical impact of pollutants on materials, thus also considering physical and environmental aspects, materials technology, chemical analytics, emission and standardization.

Environmental monitoring and evaluation of tolerability of indoor environment in the Baroque Library Hall of the National Library

(J. Smolík, joint project with National Library in Prague and Norwegian Institute for Air Research, supported by Norwegian Funds (via Ministry of Finance of CR), project No. A/CZ 0046/2/0001)

The main goal of the project is detailed characterization of indoor air pollution in the Baroque Library Hall of the National Library Hall in Prague. The research is focused both on gaseous pollutants and particulate matter (PM), including the estimation of outdoor and indoor sources contribution. [Refs. 1, 20, 43, 44, 67, 68, 70, 75, 81-83, 85]

Measurements in Baroque Library Hall of the National Library Hall in Prague

Detailed characterization of particulate matter in the indoor environment of the National Library in Prague

(J. Smolík, supported by MEYS, grant No. OC09049)

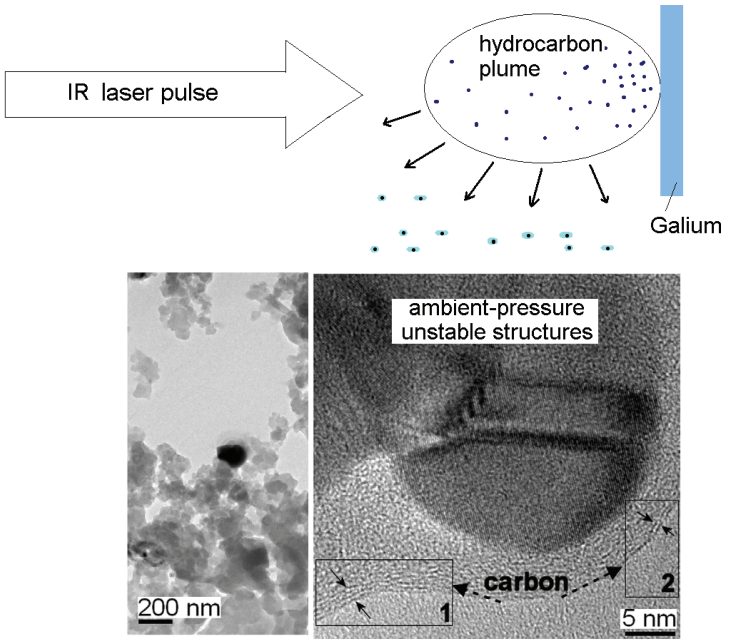
The aim of the project is detailed characterization of size-resolved PM in the indoor environment of the National Library in Prague, with possible effects on deposited books and manuscripts and estimation of contribution of typical activities indoors [Refs. 1, 36, 43, 44, 70, 75, 81-83, 85].

New laser induced process for production of novel carbon-based nanomaterials and carbon-based nanomaterials with incorporated Si, N, and B heteroatoms

(J. Pola, supported by ASCR, grant No. IAA400720619)

MW and GW UV laser-induced photolysis of gaseous benzene, toluene, pyridine and acetylene has been demonstrated as a process leading to transient polyacetylenes and cumulenes and yielding nanostructured carbon soot whose properties depend on the precursor. Simultaneous back-side etching of silica adjacent to laser-induced plasma enables to enrich the soot with polyoxocarbosilane. The process was previously shown as capable of chemical vapour deposition of composites containing nanodomains of very rare chaoite in amorphous C/Si/O/N phase, conversion of silica into nanosized carbon-polyoxocarbosilane composites, or deposition of for the first time prepared nanosized silicon oxycarbide. Our studies have been continuing in 2009 by exploration of (i) chemical vapour deposition of Co-C films through concurrent IR laser-induced ablation of metals and adjacent dielectric breakdown in gaseous hydrocarbons and (ii) studies on chemical vapour deposition of ultrafine Cl-substituted carbonaceous powders by using intense UV laser photolysis of dichloroethenes. The former process affords deposition of Co, Co_2C and Co_3C nanograins

embedded in a shell of hexagonal graphite and amorphous sp^3-hybridized carbonaceous matrix, and the latter process results in deposition of novel nanoscopic Cl-substituted hydrogenated carbon that has a potential for structural modification of carbon materials at the C-Cl bonds. [Refs. 25-29, 33, 45, 46, 54, 76]

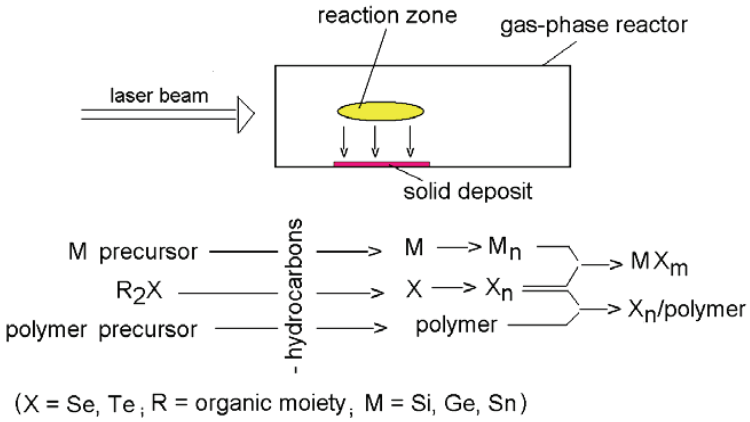


High-resolution transmission electron microscopy (HRTEM) images of the film deposited from benzene showing cubic Ga nanograins covered with curved carbon environment

Green chalcogenation of metals by laser-prepared poly(silachalcogenide)

(J. Pola, supported by GACR, grant No. GA203/09/0931

IR and UV laser co-photolysis of silane and thiirane has been studied to explore chemical vapour deposition and reactivity of poly(silathiane) towards selected metal surfaces. The poly-(silathiane) formation in the gas phase and deposition on metal surfaces was found out as a feasible process, but sulfidation of metal surfaces by this inorganic polymer reagent appears to be restricted to thin polymer-metal interphase and Cu and Bi only. Raman spectral studies confirm this conclusion. The experimental study was preceded by literature search and compiling the data on laser deposition of nanostructured Se- and Te-based materials. [Ref. 30]

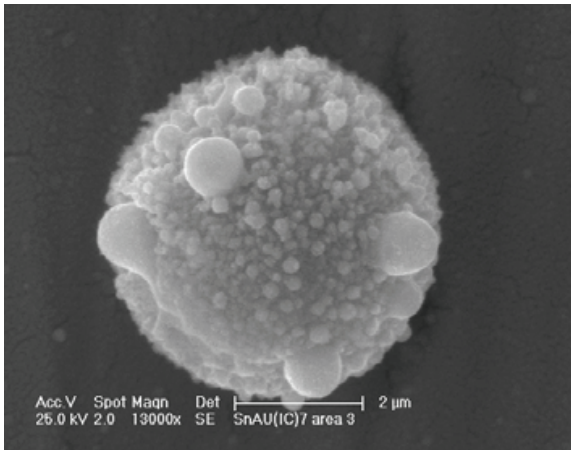


Scheme of decomposition, agglomerization and reaction/interaction between the decomposition products

IR Laser gas-phase deposition of metastable binary alloys from volatile Si, Ge and Sn precursors

(J. Pola, supported by ICPF)

IR laser-induced co-decomposition of binary gaseous mixtures of MH_4 and $M(CH_3)_4$ (M = Si, Ge, Sn) has been recognized as a novel process for gas-phase deposition of M elements alloys. The process is initiated in dielectric breakdown or by infrared multiple photon absorption in IR radiation absorbing gas and it involves extrusion and coalescence of M elements and cooling of their nanosized metastable alloys in the gas phase within short laser pulses. This one-step process represents a simple approach for synthesis of nanosized metastable alloys. [Refs. 13, 14, 24, 32, 37, 40, 57]

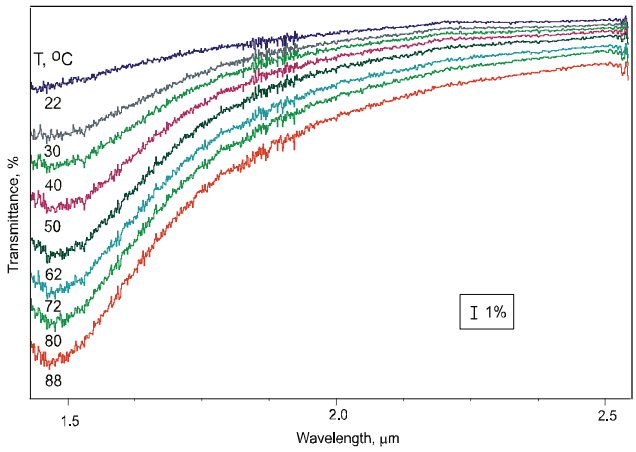


SEM of deposite obtained by laser-induced decomposition of Me_4Sn and simultaneous ablation of Au target

Preparation of Ti/O/Si based photocatalysts by laser induced CVD and sol-gel technique

(R. Fajgar, supported by GACR, grant No. GA203/09/1117)

UV laser-induced ablation of titanium and vanadium dioxide targets was used to prepare multilayer films of non-stoichiometric Ti/O/V films. The films, deposited on glass substrates were studied by means of microscopy, spectroscopy and diffraction techniques. Annealing up to 450 ^oC leads to formation of mixed-oxide layers. The films possess good adhesion to the glass substrate and revealed photochromic properties in NIR region. SnO_2/TiO_2 nanoparticles were prepared by laser-induced oxidation of tetramethyltin and titanium tetraisopropoxide. The oxidation shows an explosive course and direct formation of SnO_2/TiO_2 and SnO/TiO_2 nano-particles was observed. The nanoparticles with diameter up to 50 nm were characterized and sensoric properties were studied. [Refs. 5, 22, 38, 39]

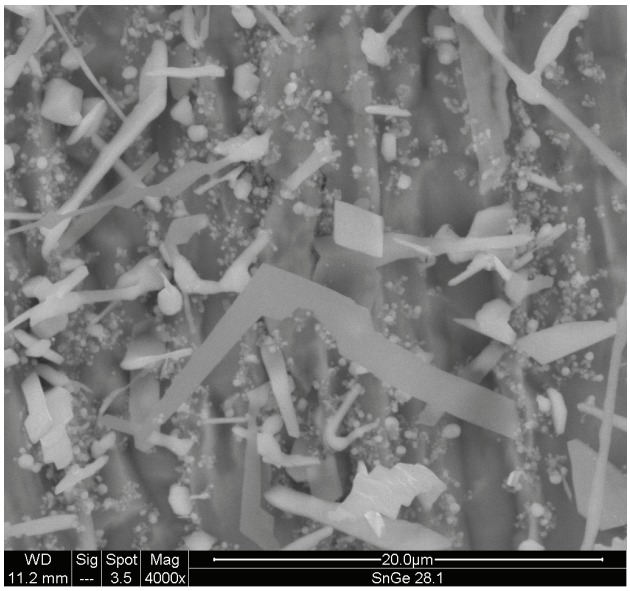


Temperature dependence of transmission spectra of the prepared Ti/O/V film in the NIR region

Preparation of nanostructured Si/Ge/C deposits

(V. Dřínek, supported by GACR, grant No. GA203/09/1088)

Nanoplatelets made of Cu_xGe_y material were prepare using Low Pressure Chemical Vapour Deposition (LPCVD) of $SnMe_4$ and Ge_2Me_6. They were represented in rhombohedral and hexagonal forms. Along with nanoplatelets, Ge nanoparticles were observed as well. They grew from CuSn seeds. Nanoplates were formed on copper sheets using precursor mixture of ethylsilane and hexamethyldigermane. The areas of nanoplates are up to thousands square microns and thickness about 50 nm. EDX analysis revealed $Cu_3Si_{0.5}Ge_{0.5}$ composition. Along with nanoplates, Cu/Si/Ge nanowires were formed. [Refs. 6, 7]



SEM picture of Cu_3Ge nanoplatelets

International co-operations

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

Division of Nuclear Physics, Department of Physics, Lund University, Lund, Sweden

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

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

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

Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, Switzerland

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
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behaviour
Philipps-Universität Marburg, Marburg, Germany: Experimental study of homogeneous nucleation in supersaturated vapours
POLYMAT, Institute for Polymer Materials, San Sebastian, Spain
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
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 Helsinki, Division of Atmospheric Sciences, Helsinki, Finland
University of Crete, Heraklion, Greece: Laser induced chemical vapour deposition of polycarbosilathianes

Visits abroad

D. Brus: Finnish Meteorological Institute, Helsinki, Finland (12 months)
J. Ondráček: Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan (1 month)

Visitors

J. Blazevska-Gilev, University of St. Cyril & Methodius, Skopje, R. Macedonia
M.A. Gondal, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia
T. Hussein, University of Helsinki, Helsinki, Finland
Nguyen Cuu Khoa, Institute of Chemical Technology, VAST, Ho Chi Minh City, Vietnam
Nguyen Thanh Danh, Institute of Chemical Technology, VAST, Ho Chi Minh City, Vietnam
V. Nororos, University of Helsinki, Helsinki, Finland
M.N. Siddiqui, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia
Ta Anh Tuan, HCM City Institute of Physics, VAST, Ho Chi Minh City, Vietnam

Teaching

V. Ždímal: Faculty of Mathematics and Physics, CU, postgraduate course: “Aerosol Engineering”
V. Ždímal: ICT, Faculty of Chemical Engineering, postgraduate course “Aerosol Engineering”

Publications

Original papers

[1] Andělová L., Smolík J., Ondráčková L., Ondráček J., López-Aparicio S., Grontoft T., Stankiewicz J.: Characterization of Airborne Particles in the Baroque Hall of the National Library in Prague. (Eng) e-Preservation Sci. 7, 141-146 (2010).

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International conferences

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12TH E. HÁLA LECTURE (2010)

RYSZARD POHORECKI (Warsaw University of Technology, Poland)
"Chemical and Process Engineering Facing the Challenges of Contemporary Civilization"

ACRONYMS USED THROUGHOUT THE REPORT

ASCR	Academy of Sciences of the Czech Republic
BAS	Bulgarian Academy of Sciences
CBM	Coal Bed Methane
CTU	Czech Technical University in Prague
CU	Charles University in Prague
EFCE	European Federation of Chemical Engineering
GACR	Grant Agency of the Czech Republic
HMS	Hexagonal Mesoporous Silica
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
IOCB	Institute of Organic Chemistry and Biochemistry of the ASCR, v. v. i., Prague
IT	Information Technology
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
MTBE	Methyl tert-Butyl Ether
NMR	Nuclear Magnetic Resonance
PBDEs	Polybrominated Diphenyl Ethers
PDMS	Polydimethylsiloxane
PM	Particulate Matter
POPs	Persistent Organic Pollutants
TU	Technical University
UJEP	Jan Evangelista Purkyně University in Ústí nad Labem
UPCE	University of Pardubice
VAST	Vietnam Academy of Science and Technology
VOCs	Volatile Organic Compounds