INSTITUTE OF CHEMICAL PROCESS FUNDAMENTALS

OF THE ASCR, V. V. I.

ANNUAL REPORT 2011

Institute of Chemical Process Fundamentals of the ASCR, v. v. i.
Prague 2012

ISBN 978-80-86186-37-5

Contents

Address Institute of Chemical Process Fundamentals
of the ASCR, v. v. i.
Rozvojová 135
165 02 Praha 6 - Suchdol
Czech Republic

GPS: 50°7'41.451"N, 14°23'0.828"E

Phone +420 220 390 111
+420 296 780 111
Fax +420 220 920 661
E-mail icecas@icpf.cas.cz
Internet http://www.icpf.cas.cz

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.

Management

Director
Jiří Hanika

Deputy Director
Olga Šolcová

Scientific Secretary
Vladimír Církva

Board of the Institute

Chairman
Karel Aim

Vice chairman
Jiří Hanika

Internal Members
Jiří Drahoš, Martin Lísal, Miroslav Punčochář, Jiří Smolík,
Olga Šolcová, Vladimír Ždímal

External Members
Josef Koubek (Faculty of Chemical Technology, ICT, Prague)
Jaromír Lederer (Institute of Inorganic Chemistry, Inc., Litvínov)
Miloš Marek (Faculty of Chemical Engineering, ICT, Prague)
Karel Ulbrich (IMC, Prague)
Kamil Wichterle (Faculty of Metallurgy and Materials Engineering,
VSB-TU, Ostrava)

Secretary
Jan Linek

SUPERVISORY BOARD

CHAIRMAN

JAN HRUŠÁK (MEYS, PRAGUE)
(UNTIL 10 SEPTEMBER 2011)
VLADIMÍR MAREČEK (ASCR)
(SINCE 11 SEPTEMBER 2011)

VICE CHAIRMAN

FRANTIŠEK KAŠTÁNEK (ICPF, PRAGUE)

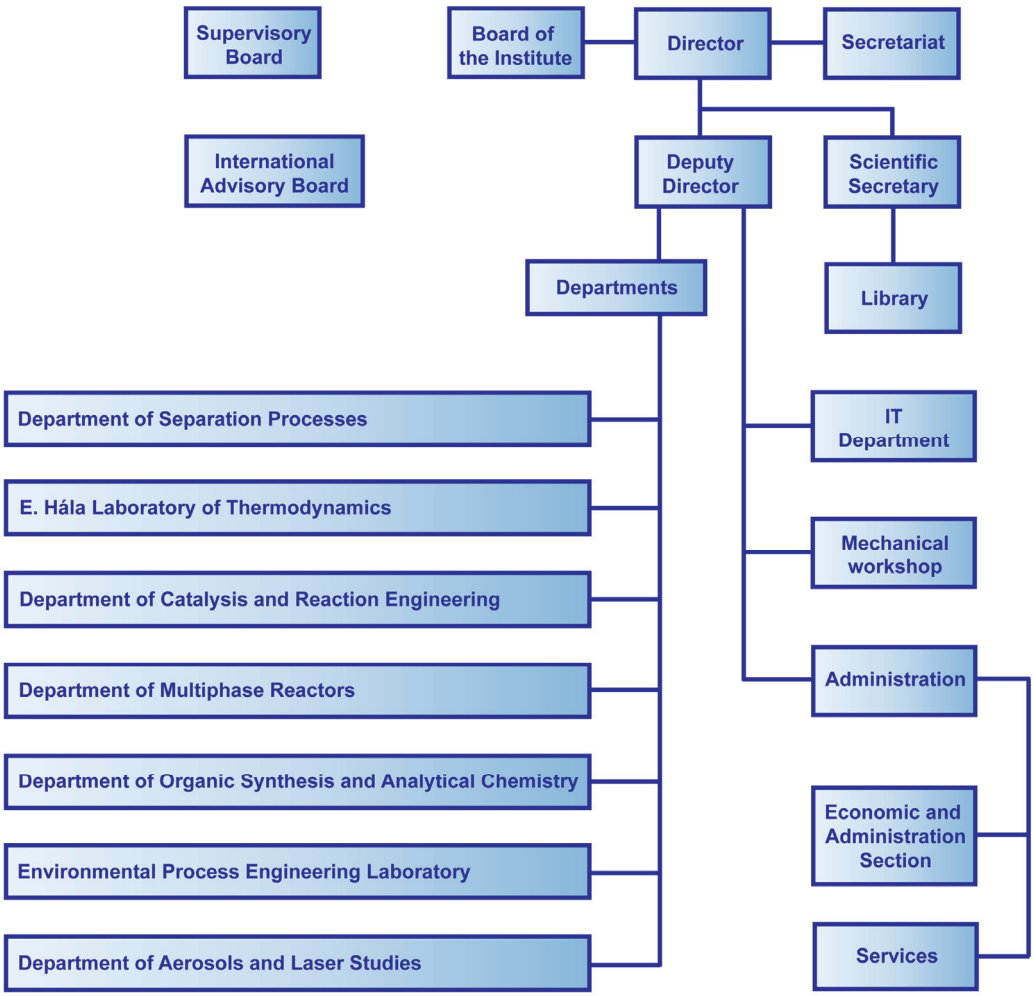
MEMBERS

KAREL BLÁHA (MINISTRY OF ENVIRONMENT OF THE CR, PRAGUE)
KAREL KLUSÁČEK (TECHNOLOGY CENTER OF THE ASCR, PRAGUE)
VLASTIMIL RŮŽIČKA (INSTITUTE OF PHYSICS OF THE ASCR, PRAGUE)

SECRETARY

VLADIMÍR CÍRKVA

Organization Chart



Administration, Secretariat and Technical Departments

Economic and Administration Section

Head
Zdeněk Novák

Deputy
Eva Krejčíková

Staff
Jan Kaura, Renáta Landová, Jana Martincová, Jana Matějovská, Renata Müllerová, Jarmila Potměšilová, Tomáš Václavek, Ilona Vachušková

Secretariat

Secretary
Alena Lvovská

Staff
Jaroslav Jíra, Iveta Kalužová, Marek Krejcar

Services

Head
Jaroslav Kratochvíl

Staff
František Červenka, Josef Holub, Jan Podzimek, Pavel Staněk

Library

Head
Eva Jirsová

Librarian
Emília Vilimovská

Mechanical workshop

Head
Jiří Goliáš

Staff
Jan Klobás, Martin Kohout, Miroslav Komm, Vladimír Kudrna, Jiří Slezák, Petr Stejskal, Vladimír Šíma

IT Department

Head
Miroslav Fridrich

Staff
David Karfík, Miloslav Strnad

STAFF

(December 31, 2011)

Category	Number of Employees
Research	150
Technical	13
Administrative	15
Services	11

BUDGET 2011

(17.60 CZK ≈ 1 US$, 24.60 CZK ≈ 1 €)

Resources	Million CZK
Institutional support based on Institutional Research Plan	94
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	62
Foreign R&D Funds and European Programmes	2
Contracts with industry	4
Total Resources	162

Expenses	Million CZK
Personal expenses including mandatory insurance	97
Purchase of material	15
Purchase of services	12
Repairs and maintenance	30
Depreciation of fixed assets	23
Travel expenses	5
Energy, water, and fuels	5
Total other expenses	12

Department of Separation Processes

HEAD
VLADIMÍR JIŘIČNÝ

DEPUTY
JIŘÍ KŘIŠŤÁL

RESEARCH STAFF
JIŘÍ HANIKA, PAVEL IZÁK, MARIE KAČÍRKOVÁ, ROMAN PETRIČKOVIČ, KRISTINA ROCHOVÁ, MILENA ROUSKOVÁ, JIŘINA ŘEZNÍČKOVÁ, MARIE SAJFRTOVÁ, PETR STAVÁREK, PETR UCHYTIL
Part time: ALEŠ HEYBERGER, KATEŘINA SETNIČKOVÁ, HELENA SOVOVÁ, VLADIMÍR STANĚK, HANA VYCHODILOVÁ

PHD STUDENTS
VERONIKA JARMAROVÁ, MAGDA KÁRÁSZOVÁ (POLONCARZOVÁ), MARKÉTA KURČOVÁ, ZUZANA VAJGLOVÁ, PETR ZÁLOHA, MAGDALENA DRHOVÁ

TECHNICAL STAFF
MARTA KOPTOVÁ, DALIBOR VLČEK
Part time: MARTIN TOPIAŘ

Fields of research

- Hydrodynamics of two phase flow in narrow channel
- Sulfur dioxide oxidation, sulfation and sulfonation
- Utilization of microreactors for enzymatic reactions
- Fluorinated hydrocarbons as potential solvents in liquid-liquid extraction processes
- Supercritical fluid extraction of biologically active substances
- Chemical and enzymatic reactions in supercritical CO_2
- Mass transport through ionic liquid membranes
- Membrane separation of methane and CO_2
- Separation of racemic mixtures
- Separation of gasoline vapors from air by supported ionic liquids membranes

Applied research

- Research and development of new methods of emulsification using microtechnology
- Hydrodynamic characterization of micromixers
- Heat and mass transfer of liquid flow in microreactors
- 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 liquid membrane

Research projects

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

(V. Jiřičný, jiricny@icpf.cas.cz; 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 will 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. Simulations with the model were used for development and design of new microreactor. New pilot plant size microreactor for SO_2 oxidation has been manufactured by KIT Karlsruhe. ICPF designed and manufactured for sulfonation and sulfation new microreactor and conducted hydrodynamic tests. [Refs. 14, 35, 36]

Research and developments of new methods of emulsification using microtechnology

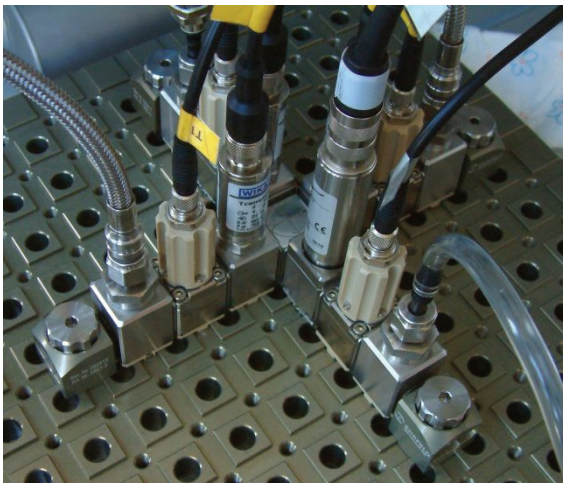
(J. Křišťál, kristal@icpf.cas.cz; contract with Procter&Gamble)

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 published in confidential Procter&Gamble research reports. [Ref. 27]

Research and developments of various microapparatus characteristics

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

The contract deals with experimental measurement of various microapparatuses (preferably mixers) and determination of their hydrodynamic characteristics with respect to various physical-chemical properties selected liquids. The collected data and developed methodology of micromixer selection will form databasis for design and development of new chemical processes. Results published in confidential Procter&Gamble research reports. [Refs. 22, 23, 45, 46]

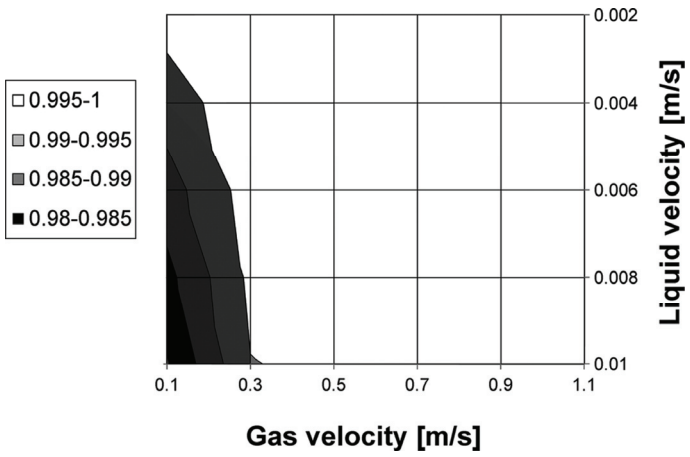


Ehrfeld micro system experimental set up for testing of micro mixers

Minimum energy dissipation under cocurrent flow in packed beds

(V. Staněk, stanek@icpf.cas.cz; supported by the GACR, grant No. 104/09/0880)

Functional analysis of mass balances on gas and liquid, and pressure drop equations describing the cocurrent flow in packed beds has yielded two criteria. The positive values of these criteria has been shown sufficient to achieve energy savings by synchronized periodic pulsations of inlet gas and liquid velocities or by the liquid velocity only compared to the situation under the same mean steady inlet phase velocities. This, however, is not the case of pulsation by gas inlet velocity alone. [Refs. 1]

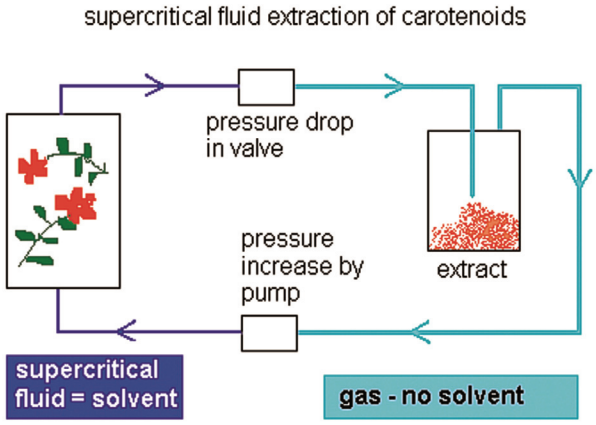


Contours of constant relative rate of energy dissipation under synchronized pulsations of liquid and gas inlet velocities for toluene/air system

Supercritical fluid extraction from vegetable materials

(H. Sovová, sovova@icpf.cas.cz; joint project with ICT Prague, Institute of Experimental Botany ASCR, Institute of Chemical Engineering of BAS, Sofia, Bulgaria; supported by MEYS, project No. 2B06024)

The sustainable use of renewable resources, complying with consumer health and environmental requirements, motivates the design, optimization, and application of green benign processes. Supercritical fluid extraction is a typical example of a novel green technology. The review offers an enumeration of extracted plant materials, discusses the mathematical modeling of the process, and advocates a choice for the appropriate model that is based on characteristic times of individual extraction steps. Finally, the attention is focused on the elements of a thermodynamic modeling framework designed to predict and model robustly and efficiently the complex phase equilibria of the systems solute+supercritical fluid. [Refs. 12, 32]



Formulation for protection of plants against insects and use thereof

(H. Sovová, sovova@icpf.cas.cz; joint project with ICT Prague, Crop Research Institute, Agra Group, a.s.; supported by MEYS, project No. 2B06049)

The solution concerns a means for the plant protection that contains a concentrate of extract from flowering aerial parts of summer savory (*Satureja hortensis* L.) in the concentration of 0.5-99.5 % wt. and at least two carriers, while at least one carrier is based on a surface active agent and/or emulsifier in the amount of 0.5-99.5 % wt. The solution concerns further the application of the insecticidal means for plant protection against insects, when the means contains at least 0.5 % wt. of the effective insecticidal substance. [Refs. 28, 30, 31, 34]

Research and development of new products for complex plant protection

(M. Sajfrtová, sajfrtova@icpf.cas.cz; joint project with Matoušek CZ a.s., Crop Research Institute; supported by TACR, project No. 01010578)

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

Mass transport during membrane permeation and pervaporation

(P. Uchytil, uchyt@icpf.cas.cz; joint project with University of Colorado, Boulder, USA; supported by MEYS, KONTAKT project No. ME 889)

Solubility, diffusivity and permeability of toluene vapors in a low-density polyethylene (LDPE) membrane of various thicknesses (approximately 48, 93, 138 and 187 μm) at different temperatures 30, 40 and 50 °C in the range of vapor relative pressure p/p^0 = (0.05; 0.95) were measured using new type of permeation apparatus. Moreover, special construction of the new cell enables determination of the permeant amount sorbed in the membrane in the steady state of the vapor permeation process. [Ref. 6]

The simple semi-empirical model of toluene transport in a polyethylene membrane based on relation between experimentally obtained effective diffusion coefficients and concentration dependent diffusion coefficients evaluated from experiments on new permeation apparatus was proposed. The model enables estimation of toluene fluxes, sorption in the steady state of vapor permeation and concentration profiles in a polyethylene membrane from equilibrium sorption isotherms and effective diffusion coefficients. Very good agreement between experimental and calculated values from the proposed model was obtained. [Ref. 11, 33]

The flow of vapors through Vycor glass membranes is investigated theoretically and experimentally. The mass flow is measured for a range of pore diameters between 20 and 200 nm and for a range of upstream conditions and pressure differences. Attention is paid to accurately describe the flow if condensation occurs. An isothermal description of the flow is found to be not sufficient. The flow of a fluid through a porous membrane constitutes a Joule-Thomson process. A vapor is cooler at the downstream side of the membrane than at the upstream side. Hence, the vapor may not only condense due to capillary condensation, but also due to heat conduction in downstream direction. The balances of mass, momentum and energy are used to describe the flow as a one-dimensional, adiabatic throttling process. The porous medium is modeled as a bundle of equivalent capillaries. Momentum transport by viscous and by molecular flow is taken into account. An expression for a characteristic pore size is given. It is found that condensation does not have a noticeable influence on the mass flow for membranes with pores larger than the characteristic pore size. The agreement between the present description and experimental data is qualitatively good and quantitatively moderate. [Ref. 5]

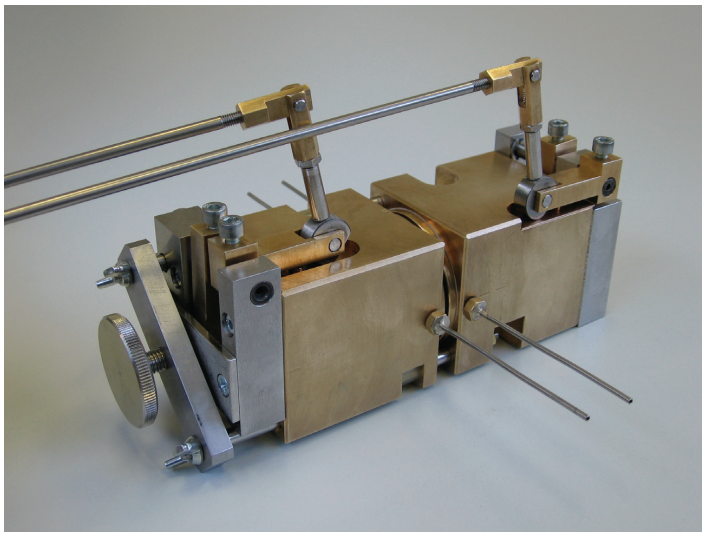


Photo of a new type of the permeation cell for determination of transport parameters in polymeric membranes

Liquid layers immobilized between nanoparticles-filled membranes for gas separation

(P. Uchytil, uchyt@icpf.cas.cz; joint project with National Chung Hsing University, Taiwan; supported by ASCR and by National Science Council of Taiwan, project No. 106/10/J038)

Polyethersulfone (PES)-based mixed matrix membranes (MMMs) with the incorporation of inorganic fillers of different shapes (Na-montmorillonite (MMT) clays and TiO_2 nanoparticles) were prepared in this study, and separation of carbone dioxide and methane was studied. It was observed that gas permeabilities increased significantly with the increasing filler content and consequently the gas selectivity was greatly reduced. At high MMT loadings (10 and 20 wt%), Knudsen diffusion became the predominant gas transport mechanism. A different trend was achieved in the case of PES/TiO_2 MMMs. The CO_2/CH_4 separation factor increased from 24.5 (pure PES membrane) to 38.5 for 4 wt% TiO_2 MMM and then decreased with a further increase in TiO_2 content (17.3 for 20 wt%). The formation of interface voids and the enlarged layer spacing of MMT clays in MMMs should have contributed to the high gas permeabilities and low gas selectivity. Moreover, inorganic filler agglomeration became serious at high loading cases and resulted in worse gas separation performance. We used also these membranes for testing transport properties of ionic liquids. [Refs. 13, 24, 40]

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

(P. Uchytil, uchyt@icpf.cas.cz; joint project with IMC, supported by the GACR, grant No. 104/09/1165)

Pervaporation transport of binary mixtures of four butanol isomers (1-butanol, 2-butanol, isobutanol and *tert*-butanol) with water through polyethylene membrane was studied. The pervaporation experiments were performed with binary mixtures of the large concentration range of butanol in water which is limited by their mutual miscibility expect of *tert*-butanol. The effect of temperature, feed concentration and the shape of the permeating species on pervaporation characteristics is investigated. In spite of the ability of butanols to form hydrogen-bonds through their hydroxyl groups and therefore to form clusters in liquid feed, with respect to hydrophobic character of polyethylene membrane the strong influence of the water on the butanol isomers transport was not expected. [Ref. 25]

The obtained results are interesting-diffusion coefficients with increasing of water concentration in the binary mixtures were increasing. Permeation fluxes were decreasing strongly for 10 wt. % of water in comparison with pure butanols – around 40 wt. % but for higher content of water in mixtures till 90 wt. % they remained practically constant. By comparing permeance of butanols, we found that the permeance of studied butanol isomers followed the following order: 2-butanol > 1-butanol > isobutanol > *tert*-butanol. To better understand these results it will be necessary to do additional experiments (i.e. with mass spectrometer) with the study of water transport. Study of transport properties of pervaporation membranes on the basis of poly-γ-benzyl-L-glutamate was published. [Ref. 4]

Ionic membranes for selective separation of liquid mixtures by pervaporation

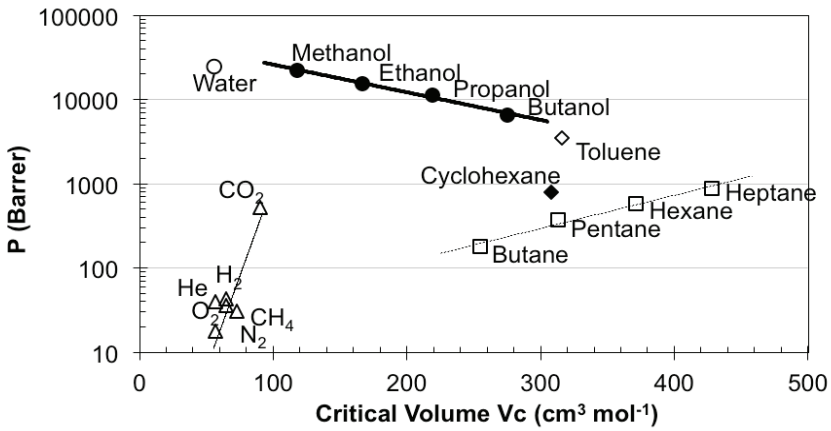
(P. Izák, izak@icpf.cas.cz; joint project with ICT Prague; supported by GACR, grant No. 104/08/0600)

Ionic liquids seem to have a large potential in downstream processing, especially when applied in a form that requires only a small amount of them, e.g. in supported liquid membranes. The special property of ILs is their non-measurable vapor pressure that makes their application in liquid membranes attractive for pervaporation. The objective is to investigate the development and application of supported liquid membranes on the base of ionic liquids. The project will be focused on products of biotransformation, waste water treatment and other valuable products, where practical application in industry is ensured. [Ref. 8, 19, 20]

Separation of volatile organic compounds (VOCs) from air

(P. Izák, izak@icpf.cas.cz; joint project with ICT Prague; supported by GACR, grant No. 106/10/1194)

The aim of this project is a development and application of membrane techniques to increase the affectivity of classical separation processes with help of computer simulations and theoretical modeling. In most of processes the goal of separation techniques is to recycle vapor phase which was lost in a sweeping gas. The optimization of polymeric membrane for specific separation task is time consuming and financial demanding. Ionic liquids have a great potential for membrane processes especially if only a small amount of ionic liquid is necessary e.g. supported ionic liquid membranes (SILMs). Characteristic property of ionic liquid is their very low vapor pressure which makes them attractive for gas and vapor permeation. [Ref. 3, 16, 18]



Permeability of supported ionic liquid membrane on critical volume of permeating molecules

Effective purification of biogas by condensing-liquid membrane

(P. Izák, izak@icpf.cas.cz; joint project with Czech head)

Currently, the biogas upgrading is widely discussed topic and because of shortening resources of fossil fuels it will remain. Biogas is easily accessible renewable fuel. Today biogas is mostly used in combined heat and power production plants however the electricity from these plants will not be so advantageous in the future because of limited capacity of the system. Biomethane as the substitute for natural gas will soon be necessary to keep our level of living. Much more progress is necessary for development of new and effective processes for biogas upgrading.

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 continuously refreshed water layer in a hydrophilic porous membrane. The permeation flux of each component of biogas depends on the feed flow rate of the gases and pressure and temperature differences between the upstream and downstream side of the condensing-liquid membrane. Selectivity increases with a lower feed flow rate. The molar balance based on 43 linear equations confirmed the high potential of this method to upgrade raw biogas. The condensing-liquid membrane can also be used under unfavorable conditions in which other polymeric membranes could be contaminated or destroyed by aggressive substances. [Refs. 7, 15, 21, 26]

International co-operations

CNRS Toulouse, France: Characterization of two phase flow in microchannels
CNRS Lyon: Hydrogenation in falling film microreactor
KIT Karlsruhe: Design of pilot plant size microreactor for sulfur dioxide catalytic heterogeneous oxidation
Procter&Gamble: Hydrodynamics of micro reactor for sulfonation
CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials
Institute of Chemical Engineering, Sofia, BAS: 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/vapor and vapor/vapor separations
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 vapors through porous membranes
Technical University of Lisbon, Portugal: Supercritical extraction of biological compounds from aromatic plants
University of Colorado, Boulder, CO, USA: Mass transport during vapor permeation and pervaporation, ionic liquids
University of Burgos, Spain: Enzymatic reactions of oil in supercritical CO_2 medium

University of KwaZulu-Natal, Republic of South Africa: Liquid-liquid extraction processes with fluorinated hydrocarbons

Visits abroad

J. Křišťál: Procter & Gamble, Brussels, Belgium (3 months)
P. Záloha, CNRS, Toulouse, France (2 weeks)
P. Uchytil, National Chung Hsing University, Taichung, Taiwan (3 weeks)

Visitors

J. Aubin, CNRS Toulouse, France
A. Bucić-Kojić, Faculty of Food Technology, Osijek University, Croatia
M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
A. Palavra, Technical University of Lisbon, Portugal
V. Villar, ENSIASET, Toulouse, France
V. Rochatte, 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] Akramov T.A., Stavárek P., Jiřičný V., Staněk V.: Minimum Energy Dissipation under Cocurrent Flow in Packed Beds. *Ind. Eng. Chem. Res.* 50(18), 10824-10832 (2011).

[2] Hanika J., Lederer J., Tukač V., Veselý V., Kováč D.: Hydrogen Production via Synthetic Gas by Biomass/Oil Partial Oxidation. *Chem. Eng. J.* 176-177(1), 286– 290 (2011).

[3] Jensen J., Friess K., Clarizia G., Schauer J., Izák P.: High Ionic Liquid Content Polymeric Gel Membranes: Preparation and Performance. *Macromolecules* 44(1), 39-45 (2011).

[4] Kononova S.V., Kremnev R.V., Baklagina Yu.G., Volchek B.Z., Vlasova E.N., Shabsels B.M., Romashkova K.A., Romanov D.P., Arkhipov S.N., Bogomazov A.V., Uchytil P.: Interrelation between the Structural and Transport Properties of Pervaporation Membranes with Diffusion Layers Based on Poly-γ-Benzyl-L-Glutamate. *Crystallogr. Rep.* [*Kristallografiya*, 56(3), 538-544, 2011] 56(3), 502-507 (2011).

[5] Loimer T., Uchytil P., Petričkovič R., Setničková K.: The Flow of Butane and Isobutene Vapors Near Saturation Through Porous Vycor Glass Membranes. *J. Membr. Sci*. 383(1-2), 104-115 (2011).

[6] Petričkovič R., Setničková K., Uchytil P.: New Apparatus for Gas Permeability, Diffusivity and Solubility Assessing in Dense Polymeric Membranes. *J. Membr. Sci.* 369(1-2), 466-473 (2011).

[7] Poloncarzová M., Vejražka J., Veselý V., Izák P.: Effective Purification of Biogas by Condensing-Liquid Membrane. *Angew. Chem.-Int. Edit.* 50(3), 669-671 (2011).

[8] Randová A., Bartovská L., Hovorka Š., Izák P., Friess K., Janků J.: Sorption of Binary Mixtures of Toluene plus Lower Aliphatic Alcohols $C_1 - C_6$ in Low-Density Polyethylene. *J. Appl. Polym. Sci.* 119(3), 1781-1787 (2011).

[9] Rousková M., Heyberger A., Tříska J., Krtička M.: Kapalinová extrakce fytosterolů a dalších cenných látek z tálových mýdel. Liquid-Liquid Extraction of Phytosterols and Other Valuable Compounds from Tall Soap. *Chem. Listy* 105(4), 251-255 (2011).

[10] Rousková M., Heyberger A., Tříska J., Krtička M.: Extraction of Phytosterols from Tall Oil Soap Using Selected Organic Solvents. *Chem. Pap.* 65(6), 805-812 (2011).

[11] Setničková K., Wagner Z., Noble R., Uchytil P.: Semi-Empirical Model of Toluene Transport in Polyethylene Membranes Based on the Data Using a New Type of Apparatus for Determining Gas Permeability, Diffusivity and Solubility. *Chem. Eng. Sci.* 66(22), 5566-5574 (2011).

[12] Sovová H., Stateva R.P.: Supercritical Fluid Extraction from Vegetable Materials. *Rev. Chem. Eng.* 27(3-4), 79-156 (2011).

[13] Uchytil P., Schauer J., Petričkovič R., Setničková K., Suen S.-Y.: Ionic Liquid Membranes for Carbon Dioxide-Methane Separation. *J. Membr. Sci.* 383(1-2), 262-271 (2011).

Chapters in books

[14] Evans J.W., Jiřičný V.: Chapter 16: Spouted Bed Electrochemical Reactors. (Eng) In: Spouted and Spout -Fluid Beds: Fundamentals and Applications. (Epstein N. - Grace J.R., Ed.), pp. 269-282, Cambridge University Press, New York 2011.

[15] Kárászová M., Friess K., Šípek M., Jansen J.C., Izák P.: Biogas: Production, consumption and applications. In *Biogas upgrading for the 21st century*. (Litonjua R., Cvetkovski I., Ed.), Nova Science Publishers, New York 2011.

[16] Friess K., Izák P., Šípek M., Jansen J.C.: Transport of VOCs in Polymers. In: *Volatile Organic Compounds*. (Columbus F., Ed.), Nova Science Publishers, New York 2011.

Patents

[17] Gruber V., Rousková M., Heyberger A., Staf M.: Způsob získávání extraktů s obsahem europia a yttria. (Czech) Method for Reclaiming of Organic Extracts Containing Europium and Yttrium Ions. Pat. No. CZ302854/PV 2010-928. Applied: 10.12.14, patented: 11.12.14.

International conferences

[18] Friess K., Jansen J.C., Clarizia G., Bernardo G.P., Bazzarelli G.F., Schauer J., Jarmarová V., Kačírková M., Izák P.: Separace plynů a par pomocí fluoropolymerních membrán s vysokým obsahem iontové kapaliny. (Czech) Separation of Gases and Vapours by High Ionic Liquid Content Fluoropolymer Membranes. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 40 (A2.3), Srní, Šumava, Czech Republic, 24-27 October 2011.

[19] Kačírková M., Randová A., Hovorka Š., Schauer J., Tisma M., Izák P.: How Ionic Liquid Changes Properties of Dense Membrane in Pervaporation Separation Process? 25th European Symposium on Applied Thermodynamics , Book of Abstracts, p. 40, Saint Petersburg, Russia, 24-27 June 2011.

[20] Kačírková M., Žitka J., Sysel P., Štorch N., Izák P.: Membránové dělení racemických směsí. (Czech) Membrane Separation of Racemic Mixtures. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 142 (V15), Srní, Šumava, Czech Republic, 24-27 October 2011.

[21] Kárászová M., Izák P.: Separace oxidu uhličitého od methanu kapalnou iontovou membránou. (Czech) Separation of Carbon Dioxide from Methane by Ionic Liquid Membrane. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 143 (V16), Srní, Šumava, Czech Republic, 24-27 October 2011.

[22] Křišťál J., Drhová M., Jiřičný V., Kuncová G.: Microreactor Flow System for Enzymatic Reactions. CAMURE-8 & ISMR-7, Book of Abstracts, p. 149, Naantali, Finland, 22-25 May 2011.

[23] Křišťál J., Jiřičný V., Hanika J.: Modulární mikrosystémy pro výzkum nových procesů. (Czech) Modular Microsystems for Novel Processes Research . 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, 7 pp., full text on CD-ROM, p. 51 (C2.1), Srní, Šumava, Czech Republic, 24-27 October 2011.

[24] Liang C.-Y, Petričkovič R., Uchytil P., Suen S.-Y.: Gas Separation Using PES-MMT Membrane/Ionic Liquid/PES-MMT Membrane in a Sandwich Form. International Congress on Membranes and Membrane Processes ICOM 2011, Poster Session 1, ICOM672, Amsterdam, Netherlands, 23-29 July 2011.

[25] Petričkovič R., von Langemann M., Setničková K., Uchytil P.: The Influence of Water on Butanols Isomers Pervaporation Transport through Polyethylene Membrane. 21st Annual Meeting of the North American Membrane Society, Program Book, p. Skyview 4, Las Vegas, Nevada, USA, 4-8 June 2011.

[26] Poloncarzová M., Vejražka J., Veselý V., Izák P.: Effective Purification of Biogas by a Condensing-Liquid Membrane. 38th International Conference of Slovak Society of Chemical Engineering , p. 102, Tatranské Matliare, Slovakia, 23-27 May 2011.

[27] Preziosi V., Křišťál J., Simoncelli A., Guido S.: Microstructure of Model Emulsion in Process Flow. 12th International Conference on Multiphase Flow in Industrial Plants, Conference Program, p. 43, Ischia, Napoli, Italy, 21-23 September 2011.

[28] Rochová K., Kurčová M., Sajfrtová M., Sovová H., Pavela R.: Supercritical CO2 Extraction of Biological Insecticides from Savory and Lavender. 11th International Conference on Carbon Dioxide Utilization, Program and Abstracts, p. 206, Dijon, France, 27-30 June 2011.

[29] Rousková M., Heyberger A.: Extrakce tálového mýdla vybranými organickými rozpouštědly. (Czech) Extraction of Tall Soap by Use of Selected Organic Solvents. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, p. 736-743, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

[30] Sajfrtová M., Pavela R., Karban J.: Vliv podmínek superkritické extrakce na insekticidní účinky výtažků z routy vonné. (Czech) Effect of Conditions of Supercritical Fluid Extraction on Insecticidal Activity of Isolates from Rue. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 166 (V39), Srní, Šumava, Czech Republic, 24-27 October 2011.

[31] Sajfrtová M., Rochová K., Karban J., Sovová H., Pavela R.: Supercritical Fluid Extraction of Botanical Insecticides from Rue. 11th International Conference on Carbon Dioxide Utilization, Program and Abstracts, p. 207, Dijon, France, 27-30 June 2011.

[32] Sajfrtová M., Sovová H.: High-Pressure CO_2 as a Green Solvent for Extraction, Reaction, Particle Formation and Others Processes. Biotech 2011 and 5th Czech-Swiss Symposium with Exhibition, Book of Abstracts, pp. 61-62, Prague, Czech Republic, 15-17 June 2011.

[33] Setničková K., Wagner Z., Noble R.D., Uchytil P.: Model transportu toluenu polyethylenovou membránou založený na datech aparatury nového typu. (Czech) Semi-Empirical Model of Toluene Transport in Polyethylene Membrane Based on the Data of New Type of Apparatus for Gas Permeability, Diffusivity and Solubility. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 39 (A2.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[34] Sovová H.: Zjednodušený výpočet průtočného náplňového kontaktoru pomocí charakteristických časů. (Czech) A Simplified Calculation of a Continuous Flow Packed Contactor with Help of Characteristic Times. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 70 (B3.5), Srní, Šumava, Czech Republic, 24-27 October 2011.

[35] Stavárek P., Křišťál J., Jiřičný V., Staněk V., Simoncelli A., Vanhoute D., Davison S., Haas-Santo K., Benzinger W.: Parametric Sensitivity Study of SO_2 Oxidation Model in Micro-Channels. 8th European Congress of Chemical Engineering, Programme, p. 1, Berlin, Germany, 25-29 September 2011.

[36] Stavárek P., Křišťál J., Jiřičný V., Staněk V., Simoncelli A., Vanhoutte D., Davison S., Haas-Santo K., Benzinger W.: Model of Capillary Micro-Reactor with Wall-Coated Catalyst for SO2 Oxidation. CAMURE-8 & ISMR-7, Book of Abstracts, p. 148, Naantali, Finland, 22-25 May 2011.

[37] Tukač V., Hanika J., Veselý V., Kovač D., Lederer J.: Modelování parciální oxidace olejové suspenze biomasy. (Czech) Modeling of Partial Oxidation of Biomass Oil Suspension . 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 56 (C2.6), Srní, Šumava, Czech Republic, 24-27 October 2011.

[38] Tukač V., Hanika J., Veselý V., Kovač D., Lederer J.: Simulace parciální oxidace biomasy. (Czech) Simulation of Biomass Partial Oxidation. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, p. 173-180, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

[39] Tukač V., Hanika J., Veselý V., Lederer J., Kovač D.: Simulation of Biomass Partial Oxidation. 1st International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH), Proceedings, Session 1, Poster 111, pp. 422-424, Noordwijkerhout, Netherlands, 29-31 July 2011.

[40] Uchytil P., Schauer J., Kočiřík M., Brabec L., Petričkovič R., Suen S.-Y.: Ionic Liquid Membranes - Permeability and Gas Separation. 1st International Conference on Ionic Liquids in Separation and Purification Technology, Posters, P04, Sitges, Spain, 4-7 September 2011.

[41] Vajglová Z., Vychodilová H., Kotas P., Kaštánek F., Jiřičný V.: Degradace polybromovaných difenyl éterů. (Czech) Degradation of Polybrominated Diphenyl Ethers. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, p. 698-704, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

[42] Vajglová Z., Vychodilová H., Tříska J., Kaštánek F., Jiřičný V.: Degradation Methods for Polybrominated Diphenyl Ethers in Liquid Wastes. (Eng) 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 141-145 full text on CD-ROM, Tatranské Matliare, Slovakia, 23-27 May 2011.

[43] Vajglová Z., Vychodilová H., Křišťál J., Kaštánek F., Jiřičný V.: Selected Methods of Dehalogenation of Polybrominated Diphenyl Ethers. 8th European Congress of Chemical Engineering, Programme, P05.04, Berlin, Germany, 25-29 September 2011.

[44] Veselý V., Hanika J., Lederer J., Nečesaný F., Kukačka J.: Tvorba a eliminace emisí PCDD/F při spalování odpadních plastů. (Czech) Formation and Elimination of Emissions of PCDD/F at Combustion of Waste Plastic Materials. 1st World Conference PETrA 2011 Pollution and Environment - Treatment of Air , Poster section, p. 1-6 full text on CD-ROM, Prague, Czech Republic, 17-20 May 2011.

[45] Záloha P., Křišťál J., Tigri S., Jiřičný V., Aubin J.: Hydrodynamics and Mixing of Gas-Liquid Flows in Thin-Gap Microchannels. 8th European Congress of Chemical Engineering, P07.23, Berlin, Germany, 25-29 September 2011.

[46] Záloha P., Tigri S., Křišťál J., Aubin J., Jiřičný V.: Local Hydrodynamics of Liquid and Gas-Liquid Flows in Thin-Gap Microchannels. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 108, Tatranské Matliare, Slovakia, 23-27 May 2011.

E. Hála Laboratory of Thermodynamics

HEAD
KAREL AIM

DEPUTY
MARTIN LÍSAL

RESEARCH STAFF
MAGDALENA BENDOVÁ, GROZDANA BOGDANIĆ, JAN LINEK, ALEXANDR MALIJEVSKÝ, LENKA MORÁVKOVÁ, JAN PAVLÍČEK, ZUZANA SEDLÁKOVÁ, LUKÁŠ VLČEK, ZDENĚK WAGNER, IVAN WICHTERLE
Part time: JAN JIRSÁK, IVO NEZBEDA, MILAN PŘEDOTA

PHD STUDENT
KAROLINA MACHANOVÁ, STANISLAV PAŘEZ

TECHNICAL STAFF
ADÉLA ANDRESOVÁ, SVATOSLAVA BERNATOVÁ

Fields of research

- Experimental determination and modeling of phase equilibria in fluid and condensed systems, including systems containing ionic liquids, polymers, 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 modeling and processing of thermodynamic data

Applied research

- Technology for the 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, kaim@icpf.cas.cz; joint project with UJEP and CTU, supported by ASCR, grant No. IAA400720710)

The research continued on applications of results obtained in the framework of perturbation methods. Further use was 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. A feasibility study on the use of non-Lorentz-Berthelot combining rules for water-methanol mixtures has been performed. New applications of DFT (density functional theory), in particular for studying the behavior of model colloidal fluids and phenomena at the gas-liquid interface on curved substrates, have been developed. Thermophysical properties of alkylammonium-based ionic liquids were experimentally studied over a range of conditions. [Refs. 1, 6, 7, 10, 11, 16, 18-20, 39]

Thermodynamic properties of mixtures of ionic liquids and molecular solvents for use in two-phase catalysis

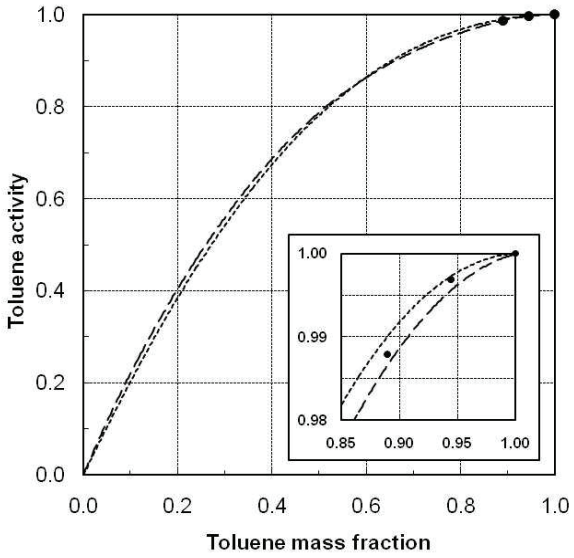
(M. Bendová, bendova@icpf.cas.cz; joint project with Institute of Microbiology of the ASCR; Zentiva Group, a.s., Prague; supported by MEYS, project No. MEB021009)

Noyori-type Ru-BINAP catalytic complexes may be used to a great advantage in syntheses of highly pure optically active compounds. Pseudo-immobilization of the catalyst by means of ionic liquid provides good contact between the catalyst and substrates. However, the contamination of ionic liquid by trace amounts of impurities may negatively affect the catalytic activity of the complex. The work is therefore aimed at optimizing the process of ionic liquids purification and their subsequent use in model asymmetric hydrogenation of methyl-3-oxobutanoate to methyl-3-hydroxyoxobutanoate in a reversibly biphasic mixture of ethanol / 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF_6]. Phase behaviour of mixtures [bmim][PF_6] with the precursors 1-chlorobutane and 1-methylimidazole as well as the efficiency of the individual purification steps were determined. [Refs. 5, 34]

Phase equilibria in the polymer-solvent systems for the design of energy-efficient separation processes

(G. Bogdanić, bogdanic@icpf.cas.cz; joint project with INA, Research and Development, Zagreb, Croatia; supported by ICPF)

Isothermal vapour–liquid equilibrium data were determined for polymer + toluene systems. Due to their importance as flow improvers for crude oil, the polymers studied were copolymers and terpolymers of octadecyl acrylate, acrylic acid, 1-vinyl-2-pyrrolidone, and styrene. Two group-contribution models (the Entropic-FV activity coefficient model, and the GC-Flory EOS) were used to predict the phase behaviour of the systems. Very good agreement with experimental data was achieved, as illustrated in the graph for poly($ODA_{0.79}$–$AA_{0.11}$–$VP_{0.10}$) terpolymer solution. Also, a new method for the estimation of porous structure parameters of crosslinked macroporous copolymers was developed. The method enables the estimation of specific pore volumes of poly(GMA-co-EGDMA) copolymers within experimental errors. Preliminary results for quick determination of liquid–liquid equilibrium in polymer solutions by the turbidimetric method were obtained for the polystyrene–methyl-cyclohexane system. [Refs. 4, 27, 29, 30, 32, 33]



Activity of toluene in poly(ODA$_{0.79}$–AA$_{0.11}$–VP$_{0.10}$) at 353.15 K; • experimental data; (- - -) prediction by the Entropic-FV model; (– – –) prediction by the GC-Flory model

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

(J. Linek, linek@icpf.cas.cz; supported by GACR, grant No. 104/09/0666)

The density and speed of sound in ethanol + isooctane, ethanol + toluene, and ethanol + isooctane + toluene systems were measured by Anton Paar instrumentation at four temperatures over the range from 298.15 to 328.15 K and the respective values of excess volumes V_m^E and adiabatic compressibility κ_S were calculated. The V_m^E and κ_S values for the binary systems were fitted to Redlich-Kister equation. The respective ternary data together with corresponding binary data were then fitted to the modified Redlich–Kister equation considering various numbers of ternary model parameters. It was found that even for the systems containing self-associating alcohol, only one ternary parameter is sufficient to describe well the ternary system. [Refs. 14, 36, 37, 38, 41, 42, 43]

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

(M. Lísal, lisal@icpf.cas.cz; joint project with University of South Bohemia in České Budějovice; supported by GACR, grant No. 203/08/0094)

Behavior of fluids in the nanospace, solid-liquid interfaces (metal oxide - aqueous solution) and nanoporous carbons (activated carbons and carbon nanotubes) was further 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 were 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. Numerical integration schemes based upon the Shardlow-splitting algorithm were presented for dissipative particle dynamics approaches at various fixed conditions. [Refs. 9, 12, 15, 21, 40, 47, 51, 52]

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

(I. Nezbeda, IvoNez@icpf.cas.cz; supported by ASCR, grant No. IAA400720802)

In 2011 a brand new and fundamental result has been obtained: It was shown that by introducing non-additive repulsive interactions it is possible to extend the excluded volume concept to systems with association, i.e. to systems whose behavior has not yet been fully understood and explained. It was shown that the augmented van der Waals equation of state based on a Yukawa reference provides better results than the SAFT-VR (statistical associating fluid theory for potentials of variable attractive range) equation of state. An invited perspective-review on the modeling of water, which also contains new results for the Henry's law constant and its anomaly, was published. Finally, the scope of the research has been extended by studies on cluster formation and its relation to Fisher-Widom lines. [Refs. 8, 10, 11, 13, 17, 18, 23, 25, 35, 44-46]

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

(Z. Sedláková, sedlakova@icpf.cas.cz; supported by GACR, grant No. 203/09/P141)

New experimental high-pressure binary and ternary data on phase equilibria and phase behaviour of systems containing hydrocarbons, carbon dioxide and ionic liquid were determined by Anton Paar densitometry and by Thar Technologies Super Phase Monitor SPM 20 apparatus. Binary data were compared both to the previously measured data by another verified apparatus in our laboratory and to the literature data. Both comparisons demonstrated good agreement within the experimental errors. High-pressure data of binary systems containing carbon dioxide and ionic liquid of imidazolium type with bistriflate anion were correlated by the Soave-Redlich-Kwong equation of state. Solid-liquid and liquid-liquid equilibria in system organic solvent + [emim][NTf_2] have also been studied. [Refs. 14, 36-38, 42, 43, 48, 49]

Phase equilibria for the design of energy-efficient separation processes (measurement and data processing)

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

Isothermal vapour−liquid equilibrium (VLE) data were measured in binary and ternary systems containing alcohol, hydrocarbon and (ether or ketone), namely: *tert*-butanol, 2-propanol, isooctane, *tert*-amyl methyl ether, 4-methyl-2-pentanone or 2,4-dimethyl-3-pentanone. The binary VLE data were correlated using the Wilson and NRTL (nonrandom two-liquid) equations by means of a new algorithm and resulting parameters were used for the calculation of phase behavior in the ternary system and for subsequent comparison with experimental data. [Refs. 2, 3, 22, 28, 31]

All glass recirculation still for VLE measurement

International co-operations

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

Institute of Condensed Matter, Ukrainian Academy of Sciences, Lviv, Ukraine: Modeling of molecular fluids at extreme conditions: Theory and applications

Institute of Physical Chemistry I. Murgulescu, Romanian Academy of Sciences, Bucuresti, 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

A. Andresová: Université François Rabelais, Tours, France, and Institut de Chimie du CNRS, Clermont-Ferrand, France (2 weeks)
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: Université François Rabelais, Tours, France, and and Institut de Chimie du CNRS, Clermont-Ferrand, France (2 weeks)
A. Malijevský: Imperial College, London, UK (2 months)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

D. Gheorghe Chiscan, Institute of Physical Chemistry I. Murgulescu, Romanian Academy of Sciences, Bucuresti, Romania
T. Abdallah, Laboratoire PCMB, Université François Rabelais, Tours, France
B. Montigny, 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 course “Experimental methods of determination of phase equilibria in fluid systems”
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, České Budějovice, courses “Lectures from physics oriented to particle and nuclear physics” and “Selected lectures from physics”
Z. Sedláková: UJEP, Faculty of Science, course “Chemical analysis”

Publications

Original papers

[1] Archer J.A., Malijevský A.: On the Interplay between Sedimentation and Phase Separation Phenomena in Two-Dimensional Colloidal Fluids. *Mol. Phys.* 109(7-10, SI), 1087-1099 (2011).

[2] Bernatová S., Pavlíček J., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of 2,2,4-Trimethylpentane, 2-Methyl-1-Propanol, and 4-Methyl-2-Pentanone. *Fluid Phase Equilib.* 307(1), 66-71 (2011).

[3] Bernatová S., Pavlíček J., Wichterle I.: Isothermal Vapor-Liquid Equilibria in the Two Binary and the Ternary Systems Composed of tert-Amyl Methyl Ether, tert-Butanol and Isooctane. *J. Chem. Eng. Data* 56(4), 783-788 (2011).

[4] Bogdanić G., Wichterle I.: Vapor–Liquid Equilibrium in Diluted Polymer + Solvent Systems. *J. Chem. Eng. Data* 56(4), 1080-1083 (2011).

[5] Černá I., Klusoň P., Bendová M., Floriš T., Pelantová H., Pekárek T.: Intensification of the Use of Ionic Liquids as Efficient Reaction Co-Solvents in Asymmetric Hydrogenations. *Chem. Eng. Process*. 50(3), 264-272 (2011).

[6] Fantoni R., Malijevský A., Santos A., Giacometti A.: Phase Diagram of the Penetrable-Square-Well Model. *Europhys. Lett*. 93(2), 26002 (2011).

[7] Fantoni R., Malijevský A., Santos A., Giacometti A.: The Penetrable Square-Well Model: Extensive versus Non-Extensive Phases. *Mol. Phys*. 109(23-24 SI), 2723–2736 (2011).

[8] Jackson G., Nezbeda I.: 8th Liblice Conference on the Statistical Mechanics of Liquids - Brno, Czech Republic, 13-18 June 2010 FOREWORD. *Mol. Phys*. 109(1, Sp.I:Sl), 1-2 (2011).

[9] Kolafa J., Lísal M.: Time-Reversible Velocity Predictors for Verlet Integration with Velocity-Dependent Right-Hand Side. *J. Chem. Theory Comput*. 7(11), 3596-3607 (2011).

[10] Krejčí J., Nezbeda I., Melnyk R., Trokhymchuk A.: Virial Coefficients and Vapor-Liquid Equilibria of the EXP6 and 2-Yukawa Fluids. *Condens. Matter Phys*. 14(2), 23004 (2011).

[11] Krejčí J., Nezbeda I., Melnyk R., Trokhymchuk A.: Mean-Spherical Approximation for the Lennard-Jones-like Two Yukawa Model: Comparison against Monte Carlo Data. *Condens. Matter Phys*. 14(3), 33005 (2011).

[12] Lísal M., Brennan J.K., Bonet Avalos J.: Dissipative Particle Dynamics at Isothermal, Isobaric, Isoenergetic, and Isoenthalpic Conditions Using Shardlow-like Splitting Algorithms. *J. Chem. Phys*. 135(20), 18 (2011).

[13] Melnyk R., Nezbeda I., Trokhymchuk A.: Vapour/Liquid Coexistence in Long-Range Yukawa Fluids Determined by Means of an Augmented van der Waals Approach. *Mol. Phys*. 109(1, Sp.I:Sl), 113-121 (2011).

[14] Morávková L., Wagner Z., Sedláková Z., Linek J.: Volumetric Behaviour of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from (298.15 to 328.15) K. Experimental Data and Correlation. *J. Chem. Thermodyn*. 43(12), 1906-1916 (2011).

[15] Moučka F., Lísal M., Škvor J., Jirsák J., Nezbeda I., Smith W.R.: Molecular Simulation of Aqueous Electrolyte Solubility. 2. Osmotic Ensemble Monte Carlo Methodology for Free Energy and Solubility Calculations and Application to NaCl. *J. Phys. Chem. B* 115(24), 7849–7861 (2011).

[16] Moučka F., Nezbeda I.: Water-Methanol Mixtures with non-Lorentz-Berthelot Combining Rules: A Feasibility Study. *J. Mol. Liq*. 159(1, Sp.I:Sl), 47-51 (2011).

[17] Nezbeda I., Jirsák J.: Water and Aqueous Solutions: Simple Non-Speculative Model Approach. *Phys. Chem. Chem. Phys.* 13(44), 19689-19703 (2011).

[18] Nezbeda I., Melnyk R., Trokhymchuk A.: Augmented van der Waals Equations of State: SAFT-VR versus Yukawa Based van der Waals Equation. *Fluid Phase Equilib*. 309(2), 174-178 (2011).

[19] Nold A., Malijevský A., Kalliadasis S.: Wetting on a Spherical Wall: Influence of Liquid-Gas Interfacial Properties. *Phys. Rev. E* 84(2), 021603 (2011).

[20] Nold A., Malijevský A., Kalliadasis S.: Critical Assessment of Effective Interfacial Potentials Based on a Density Functional Theory for Wetting Phenomena on Curved Substrates. *Eur. Phys. J. Special Topics* 197(1), 185–191 (2011).

[21] Patterson K., Lísal M., Colina C.M.: Adsorption Behavior of Model Proteins on Surfaces. *Fluid Phase Equilib*. 302(1-2), 48-54 (2011).

[22] Pavlíček J., Wichterle I.: Isothermal (Vapour + Liquid) Equilibria in the Binary and Ternary Systems Composed of 2-Propanol, 2,2,4-Trimethylpentane and 2,4-Dimethyl-3-Pentanone. *J. Chem. Thermodyn*. 45(1), 83-89 (2011).

[23] Rouha M., Nezbeda I.: Excess Properties of Aqueous Solutions: Hard Spheres versus Pseudo-Hard Bodies. *Mol. Phys.* 109(4), 613-617 (2011).

[24] Setničková K., Wagner Z., Noble R., Uchytil P.: Semi-Empirical Model of Toluene Transport in Polyethylene Membranes Based on the Data Using a New Type of Apparatus for Determining Gas Permeability, Diffusivity and Solubility. *J. Membr. Sci*. 66(22), 5566-5574 (2011).

[25] Škvor J., Nezbeda I.: Percolation Line and Response Functions in Simple Supercritical Fluids. *Mol. Phys*. 109(1, Sp.I:Sl), 133-139 (2011).

[26] Ždímal V., Smolík J., Eleftheriadis K., Wagner Z., Housiadas Ch., Mihalopoulos N., Mikuška P., Večeřa Z., Kopanakis I., Lazaridis M,.: Dynamics of Atmospheric Aerosol Number Size Distributions in the Eastern Mediterranean During the "SUB-AERO" Project. *Water Air Soil Pollut.* 214(1-4), 133-146 (2011).

International conferences

[27] Bendová M., Machanová K., Bogdanić G., Wichterle I.: Apparatus for Quick Determination of Liquid – Liquid Equilibrium in Polymer Solutions by the Turbidimetric Method. 36th International Invention Show (silver medal awarded), Katalog, p. 129, Zagreb, Croatia, 09-12 November 2011.

[28] Bernatová S., Pavlíček J., Wichterle I.: Vapour–Liquid Equilibria in Alcohol + Hydrocarbon + Ketone Systems. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, p. 303, Saint Petersburg, Russia, 24-27 June 2011.

[29] Bogdanić G., Jovanović S. M.: Estimation of the Porous Structure Parameters of the Crosslinked Macroporous Copolymers Based on Methacrylates. 36th International Invention Show (bronze medal awarded), Katalog, p. 127, Zagreb, Croatia, 09-12 November 2011.

[30] Bogdanić G., Jovanović S.M.: Estimation of the Porous Structure Parameters of the Crosslinked Macroporous poly(GMA-co-EGDMA). 1. Estimation of the Specific Pore Volume. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, pp. 304-305, Saint Petersburg, Russia, 24-27 June 2011.

[31] Bogdanić G., Pavlíček J., Wichterle I.: Enhanced Modification of the Glass Micro-Ebulliometer for Measurement of Total Pressure in Fluid Systems. 36th International Invention Show (gold medal awarded), Katalog, p. 128, Zagreb, Croatia, 09-12 November 2011.

[32] Bogdanić G., Wichterle I.: Vapor–Liquid Equilibrium in Diluted Polymer + Solvent Systems. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, pp. 301-302, Saint Petersburg, Russia, 24-27 June 2011.

[33] Bogdanić G., Wichterle I.: Vapor–Liquid Equilibrium in Diluted Polymer + Toluene Systems. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, 5 pp. full text on CD-ROM, p. 149 (V22), Srní, Šumava, Czech Republic, 24-27 October 2011.

[34] Dytrych P., Klusoň P., Floriš T., Lísal M., Slater M.: Theoretical Interpretation of Enantioselectivity Trends in (R)-Ru-BINAP Catalyzed Hydrogenation of Methylacetoacetate in the QAS Ionic Liquid Phase. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, 2 pp. full text on CD-ROM, p. 35 (C1.5), Srní, Šumava, Czech Republic, 24-27 October 2011.

[35] Jirsák J., Nezbeda I.: Towards a Molecular Theory of Hydrophobic Hydration: Hard Spheres in Primitive Water. 8th Liquid Matter Conference, Poster Abstracts p. 34 (P2.34), Wien, Austria, 06-10 September 2011.

[36] Linek J., Morávková L., Wagner Z., Sedláková Z.: Volumetric Behaviour of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from 298.15 K to 328.15 K. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, p. 386, Saint Petersburg, Russia, 24-27 June 2011.

[37] Linek J., Morávková L., Wagner Z., Sedláková Z.: Volumetric Properties of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from 298.15 K to 328.15 K. Thermodynamics 2011, Book of Abstracts, pp. 205-206, Athens, Greece, 31 August - 03 September 2011.

[38] Linek J., Morávková L., Wagner Z., Sedláková Z.: Volumetric Properties of Binary and Ternary Liquid Systems Composed of Ethanol, Isooctane, and Toluene at Temperatures from 298.15 K to 328.15 K. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 221 (pp.1159 -1170 full text on CD-ROM), Tatranské Matliare, Slovakia, 23-27 May 2011.

[39] Machanová K., Sedláková Z., Boisset A., Bendová M., Jacquemin J., Aim K.: Thermophysical Properties of Alkylammonium-Based Ionic Liquids. 19th European Conference on Thermophysical Properties, Book of Abstracts, p. 230, Thessaloniki, Greece, 28 August - 01 September 2011.

[40] Moore J.D., Izvekov S., Lísal M., Brennan J.K.: Particle Based Multiscale Modeling of the Dynamic Response of RDX. Conference of the APS Topical Group on Shock Compression of Condensed Matter , AIP Conference Proceedings, Vol.1426, pp. 1327-1240, 2011, Chicago, Illinois, USA, 26 June - 01 July 2011.

[41] Morávková L., Wagner Z., Linek J.: Volumetric Properties of Pyridine, 2-Picoline, 3-Picoline, and 4-Picoline at Temperatures Up to 328.15 K and at Pressures Up to 40 MPa. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 63 (pp. 301-307 full text on CD-ROM), Tatranské Matliare, Slovakia, 23-27 May 2011.

[42] Morávková L., Wagner Z., Sedláková Z., Aim K.: Measurement of Excess Volumes of Ternary Systems. 36th International Invention Show (silver medal awarded), Katalog, p. 132, Zagreb, Croatia, 09-12 November 2011.

[43] Morávková L., Wagner Z., Sedláková Z., Aim K.: Comparison of Excess Volumes for Two Ternary Systems Containing (Toluene + Isooctane) with Ethanol or 1- Butanol. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, pp. 389-390, Saint Petersburg, Russia, 24-27 June 2011.

[44] Nezbeda I.: Generalized excluded volume: Its origin and effects. 36th Conference of the Middle European Cooperation in Statistical Physics MECO 36, Lviv, Ukraine, 05-07 April 2011.

[45] Nezbeda I.: A new concept for augmented van der Waals equations of state. 25th European Symposium on Applied Thermodynamics, Saint Petersburg, Russia, 24-27 June 2011.

[46] Nezbeda I.: Generalized excluded volume: Its origin and effects. (Invited lecture) 32nd International Conference on Solution Chemistry, La Grande Motte, France, 28 August - 02 September 2011.

[47] Posel Z., Lísal M.: Scaling Laws for Polymers in Dissipative Particle Dynamics Revised. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 180 (V53), Srní, Šumava, Czech Republic, 24-27 October 2011.

[48] Sedláková Z., Rotrekl J., Bendová M., Vrbka P., Aim K.: Measurement of Solid–Liquid and Liquid–Liquid Equilibria in Organic System Containing Ionic Liquid [emim][NTf_2]. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, pp. 387-388, Saint Petersburg, Russia, 24-27 June 2011.

[49] Sedláková Z., Wagner Z., Aim K.: High-Pressure Phase Equilibria in Systems Containing CO_2 and Ionic Liquids. 36th International Invention Show (bronze medal awarded), Katalog, 10, p. 131, Zagreb, Croatia, 09-12 November 2011.

[50] Setničková K., Wagner Z., Noble R.D., Uchytil P.: Model transportu toluenu polyethylenovou membránou založený na datech aparatury nového typu. (Czech) Semi-Empirical Model of Toluene Transport in Polyethylene Membrane Based on the Data of New Type of Apparatus for Gas Permeability,

Diffusivity and Solubility. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 39 (A2.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[51] Smith W.R., Moučka F., Lísal M.: A Molecular Based Osmotic Ensemble Monte Carlo Simulation Method for Free Energy Solvation Curves and the Direct Calculation of Aqueous Electrolyte Solubility. 25th European Symposium on Applied Thermodynamics, Book of Abstracts, p. 27, Saint Petersburg, Russia, 24-27 June 2011.

[52] Trejos V.M., Lísal M., Nezbeda I., Smith W.R., Figueroa-Gerstenmaier S.: Thermodynamic Properties at Fixed Enthalpy for Alternative Refrigerants by Molecular Simulations. Thermodynamics 2011, Book of Abstracts, pp. 480-482, Athens, Greece, 31 August - 03 September 2011.

[53] Wagner Z., Fridrich M., Schwarz J., Ždímal V., Váňa M.: Measurement and Analysis of Near Real Time Data on Particle Size Distribution in Atmospheric Aerosol. 36th International Invention Show (gold medal awarded), Katalog, p. 130, Zagreb, Croatia, 09-12 November 2011.

[54] Wagner Z., Fridrich M., Schwarz J., Ždímal V.: Zpracování hromadných dat distribuce velikosti aerosolových částic v reálném čase a jejich prezentace v evropských i celosvětových databázích. (Czech) Analysis of Near Real Time Data on Particle Size Distribution in Atmospheric Aerosol and Their Presentation in International Databases. TeXperience 2011 (4.ročník) a Stakan 2011 (6.ročník), Kniha abstraktů dvoukonference, pp. 33-34, Železná Ruda, Czech Republic, 20 September - 02 October 2011.

Department of Catalysis and Reaction Engineering

HEAD
OLGA ŠOLCOVÁ

DEPUTY
PETR KLUSOŇ

RESEARCH STAFF
LIBUŠE HANKOVÁ, VLADIMÍR HEJTMÁNEK, LADISLAV HOLUB, KVĚTUŠE JIRÁTOVÁ, LUDĚK KALUŽA, JAN KLEMPA, YWETTA MALÉTEROVÁ, MARTINA MATĚJKOVÁ, LENKA MATĚJOVÁ, ROBERT PONEC, KAREL SOUKUP, HANA ŠNAJDAUFOVÁ, PAVEL TOPKA, ZDENĚK VÍT
Part time: JANA BALABÁNOVÁ, JANA GAÁLOVÁ, DANIELA GULKOVÁ, KAREL JEŘÁBEK, JAROMÍR JIRKOVSKÝ, FRANTIŠEK KAŠTÁNEK, PETR KAŠTÁNEK, HANA KMENTOVÁ (ŽABOVÁ), JOSEF KRÝSA, PETR SCHNEIDER, KRASIMIRA SOUKUPOVÁ, MIROSLAV ZDRAŽIL

PHD STUDENTS
PAVEL DYTRYCH, SIMONA KREJČÍKOVÁ, PAVEL KRYSTYNÍK, JANA LUDVÍKOVÁ, MAGDALENA MOROZOVÁ, LUCIE SPÁČILOVÁ

TECHNICAL STAFF
Part time: BARBORA PAPEŽOVÁ, HELENA SOUČKOVÁ

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
- Preparation and characterization of the electrospun nanofibrous membranes and catalytic supports
- Unconventional preparation of metal oxide nanostructures by pressurized fluid extraction and supercritical drying

Applied research

- Catalytic combustion of volatile organic compounds
- Oxidation processes for environment
- Textural characteristics of structural materials

Research projects

Hydrogen Oriented Underground Coal Gasification (UCG) for Europe - Environmental and Safety Aspects (HUGE2)

(O. Šolcová, solcova@icpf.cas.cz; supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2011-00002)

This project is focused on safety and environmental aspects of underground coal gasification. Underground trial will be performed in mine testing two borehole system and reactive barriers usage. The most serious environmental concerns related to UCG will be investigated that is contamination of underground aquifers and potential leakage of poisonous and explosive gates into the surrounding strata. The work will be focused on finding practical solutions of possible leakages prevention by use of reactive barriers. Complex system of environmental telemetric monitoring will be built and tested. Also technical and ecological risk assessment will be performed. [Refs. 23, 83]

Hierarchic nanosystems for microelectronics

(O. Šolcová, solcova@icpf.cas.cz; 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, grant No. KAN400720701)

Project developed the complex composite systems with precisely defined performance applicable in microelectronics. Prepared composite structures - various types of hierarchical nanostructures were designed, produced and functionally described, with direct implications in many types of advanced sensors; long-life humidity sensor, photoelectric gas sensor, oxalic acid sensor, etc. [Refs. 2, 11, 12, 16-18, 25, 26, 59, 64-66, 68, 69, 72, 73, 86]

Advanced photocatalytic processes - nanotechnology for environment

(O. Šolcova, solcova@icpf.cas.cz; joint project with Institute of Microbiology of the ASCR, v. v. i., and UPa; supported by GACR, grant No. 104/09/0694)

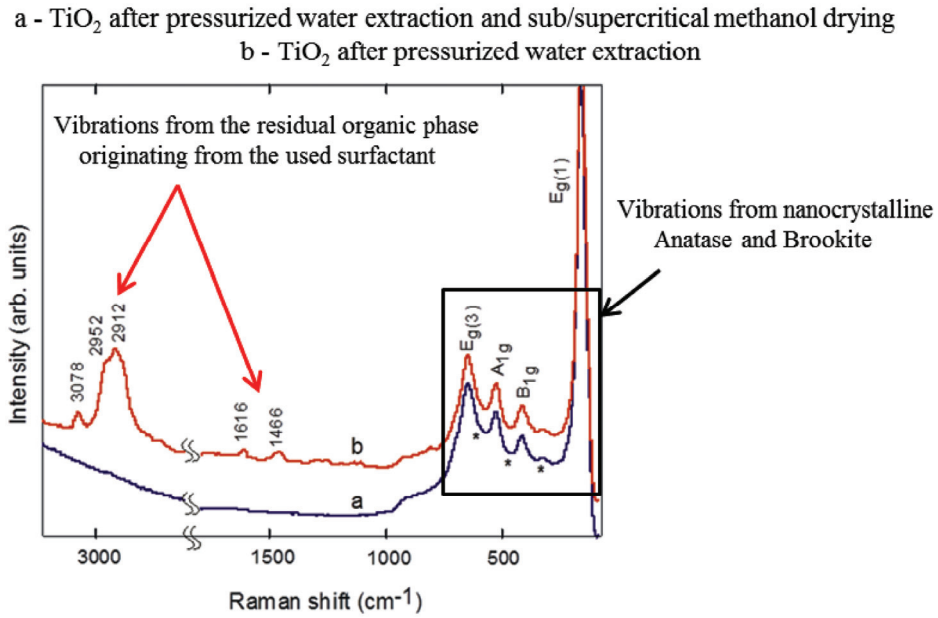
This project was focused on preparation and characterization of specially designed photoactive materials applied for decomposition of the large series of potential water contaminants ranging from phenols, chlorinated phenols, polybrominated diphenyl ethers and alcohols to herbicides, pesticides, pharmaceuticals, industrial colorants, pigments and dyes. The special focus was devoted to the reactor system; selectively prepared photoactive nanostructures together with design of effective photoreactors including mathematical modeling of involved physical and chemical processes and generalization of obtained results. [Refs. 6, 12, 17, 18, 25, 26, 58, 60, 70, 74, 75, 81, 85]

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

(L. Matějová, matejova@icpf.cas.cz; joint project with CU; supported by GACR, grant No. 104/09/P290)

Project deals with development and optimization of extraction technique for purification and total crystallization of prepared oxidic materials with high-ordered mesoporous structure. Developed extraction technique using fluids in supercritical and subcritical state will be generally applicable for synthesis of nanocrystalline metal oxides. The optimal experimental conditions (temperature, pressure, flow rate, etc.) as same as the suitable solvents will be 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 microelectronics will be synthesized by templating using amphiphilic and ionic surfactants in aqueous and alcoholic solution with metal chloride and alkoxide. [Refs. 25, 33, 65-69]



Raman spectra of nanocrystalline TiO_2 prepared by extraction techniques

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

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

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, physical-chemical properties and activity of the resulting mixed oxides in ethanol oxidation was examined in detail. Catalysts containing Co-Mn-Al over TiO_2 support with various active metals distribution were prepared in order to study the effect of metals distribution on catalyst activity in ethanol oxidation. [Refs. 14, 15, 45, 46, 61-63]

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

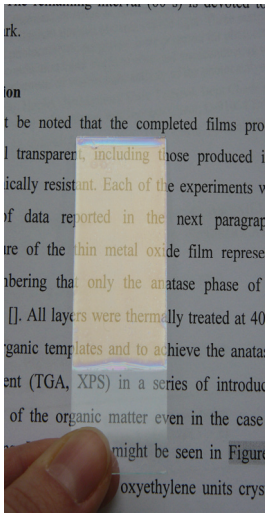
(K. Jirátová, jiratova@icpf.cas.cz; joint project with TU of Ostrava, and ICT; supported by TACR, grant No. 010220336)

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 in detail. Potassium was found to be the best promoter of the catalyst. In addition, the effect of active metals distribution in the Co-Mn-Al/TiO_2 catalysts on catalytic properties was investigated. Abatement of N_2O in waste by its decomposition over K-promoted Co-Mn-Al mixed oxide catalyst was simulated. [Refs. 19, 52, 53, 77]

Advanced catalytic processes and materials

(J. Hanika, O. Šolcová, hanika@icpf.cas.cz, solcoca@icpf.cas.cz; joint project with JH IPC, ICT, CU, and UPa; supported by GACR, grant No. 203/08/H032)

Development of the new selective catalytic and separation processes for preparation of specialty compounds and materials, which can give rise to a progression in the field of new chemical technologies was realized. The special focus was devoted to processes in question; stereoselective and regioselective transformations on chiral catalytic centers and processes with significant environmental impact. The project theses were coordinated in the field of catalysis, e.g., developed Rh catalysts were tested in stereospecific polymerizations (CU), asymmetric synthesis (ICT) and hydrocarbonylations; oxidation catalysts were tested in organic synthesis (ICT, UPa, ICPF), oxidation polymerization (CU) and synthesis of chemical specialties (JH IPC); new mesoporous materials prepared at JH IPC were used in all other partner laboratories, etc. [Refs. 8, 12, 17, 18, 57, 61-63, 71-75]

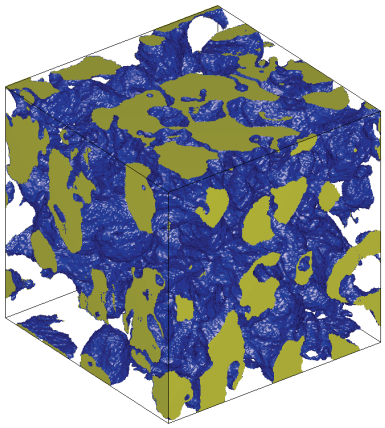


The thin transparent TiO_2 layer on glass

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

(V. Hejtmánek, hejtmanek@icpf.cas.cz; joint project with JH IPC, and ICT; supported by GACR, grant No. 203/09/1353)

The principal project goal, i.e. a development of preparation procedure for polyimide (PI) based composites with different content of microporous inclusions (silicalite–1, ZIF–8), was fulfilled. The application of a coupling species APTES enhanced mechanical stability of composites and prevented void formation at interface boundary and thus deterioration of separation factor. Prepared materials were suitable for a fundamental study of relation between macroscopic properties of the heterogeneous material on one side and microscopic descriptors of the material, self-diffusion coefficients of the gases and their occurrence probability in either phase on the other. 3D models of composite membranes microstructure were constructed using the method of stochastic reconstruction developed in the first project stage. The obtained replicas were used to simulate mass transport in the composites using a Monte Carlo algorithm. Another novel technique used in this project is the preparation procedure of polyamic acid (PAA which is the precursor of PI) based films and membranes on solid preferentially porous supports, which involves the electrophoretic deposition (EPD) of PAA solution from its emulsion in acetone. [Refs. 1, 34, 42]

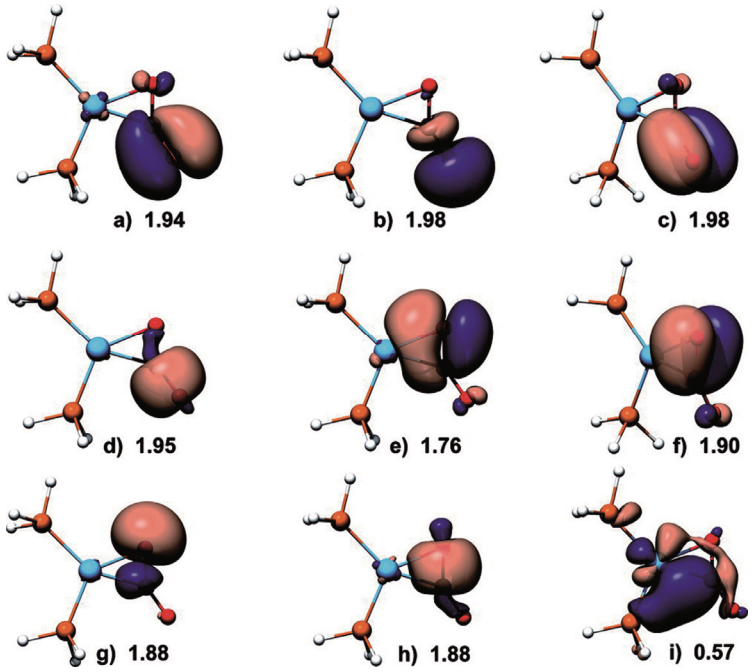


The zeolite-polyimide membrane replica (64×64×64 μm). Polyimide phase is transparent, polyimide-silicalite interface is blue and intersections of the silicalite phase and the cut planes are yellow

Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, rponec@icpf.cas.cz; joint project with University of Pécs, Hungary, Univerzity of Girona, Spain; 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 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, multicenter 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. 7, 21, 30, 31, 78-80]

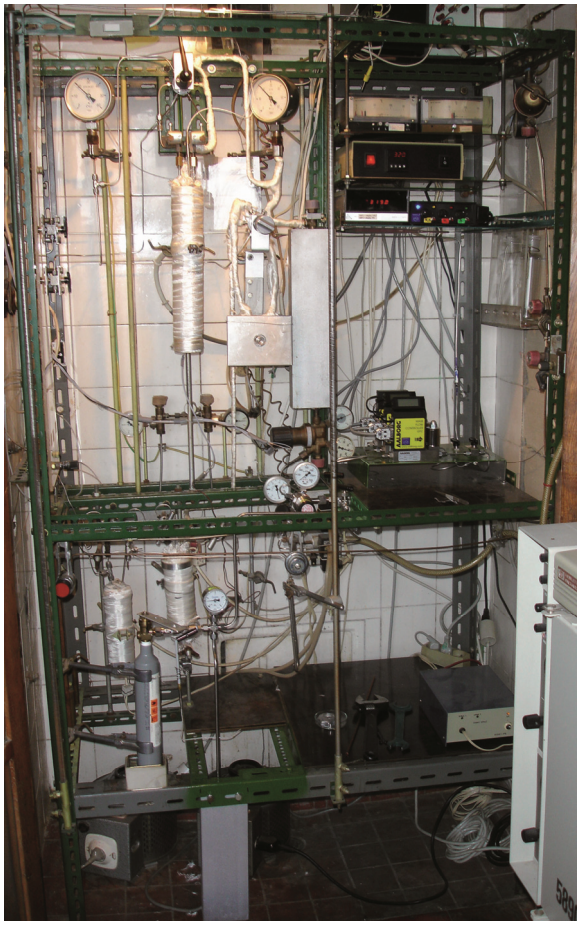


Graphical representation of the eigenvectors of the DAFH of the CO_2 fragment with the corresponding eigenvalues

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

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

Alternative acidic supports and active phases based on noble metals were studied for hydrodesulfurization (HDS) of model compounds such as thiophene and benzothiophene. Mesoporous silica-aluminas modified by acid extraction were studied as supports of Pd and bimetallic Pd-Pt catalysts. The acid extraction led to higher accessible surface areas and exposed the Brønsted acid sites of supports which both improved the HDS activity of catalysts. HDS activity was also greatly influenced by the precursor of noble metal. The inhibition effects of pyridine and toluene on HDS of thiophene was studied on sulfided Rh, Ru, Mo, Rh-Mo, Ru-Mo and CoMo/alumina catalysts. Noble metal catalysts were generally less sensitive to pyridine inhibition than conventional CoMo catalysts. Their higher nitrogen tolerance was related to higher C-N bond hydrogenolysis activity. Comparative inhibition with toluene confirmed that poisoning of conventional Mo and CoMo catalysts is due to basicity of inhibitor while not to its aromatic character. [Refs. 27, 28, 38, 39, 91, 92]



Pressure flow microreactor with fixed bed of catalyst for hydrodesulfurization

Functional macroreticular polymers as catalyst carriers

(K. Jeřábek, kjer@icpf.cas.cz; joint project with Department of Chemical Sciences, University of Padova, 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. There was developed a feasible method for modification of chemical nature of ion exchanger catalyst for applications in processes involving lipophilic reagents. [Refs. 29, 32, 40, 43, 44]

Post-polymerization hypercrosslinking of monolytic polymers

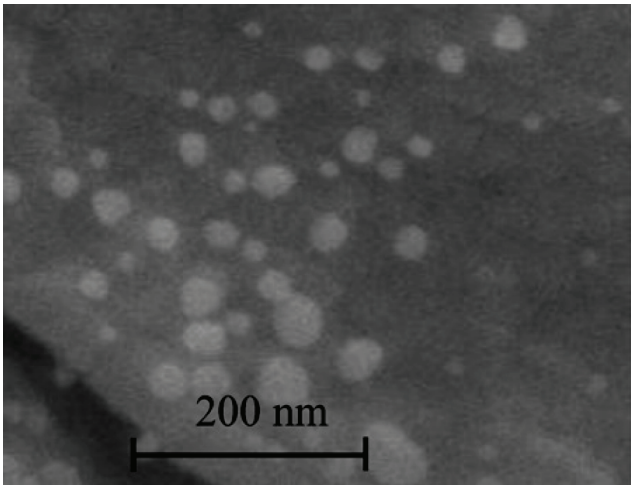
(K. Jeřábek, kjer@icpf.cas.cz; joint project with University of Maribor, Slovenia, supported by MEYS, grant No. MEB091107)

Within this project are investigating possibilities of modifications of morphology of monolytic porous polymers by additional crosslinks introduced to the already polymerised monolithic material. In this manner, much smaller pores are created thus significantly enlarging the surface area while leaving the larger pores intact. [Refs. 13, 41]

New catalysts for VOC oxidation

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

Novel oxidation catalysts based on noble metals supported on ceria-zirconia mixed oxides were developed, characterized and their catalytic activity in total oxidation of model volatile organic compounds was studied. In collaboration with the Finnish partner, platinum and gold catalysts with noble metal content in the range from zero to 2.5 wt. % were tested in total oxidation of dichloromethane. Their physicochemical properties (dispersion of noble metal, reducibility, acidobasic properties) were correlated with their catalytic performance and activity/selectivity vs. composition/structure relationships were proposed. [Refs. 20, 36, 37, 47]



Gold nanoparticles on ceria-zirconia support as seen by field-emission scanning electron microscope

Development of oxide catalysts for total oxidation of ethanol

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

The second year of the project was focused on catalytic testing of newly developed catalysts in the oxidation of ethanol. The results of the project revealed that ceria-zirconia mixed oxides exhibited high activity and low formation of undesired reaction by-products. Novel catalysts were prepared by doping of ceria-zirconia with noble metals. It was shown that the addition of gold and platinum can dramatically affect the efficiency of the catalysts.

The effect of metal content and metal dispersion was investigated and correlated with activity and selectivity of the catalysts. Except the experiments with powder catalysts, new methods for the synthesis of monolithic catalysts were proposed and tested. [Refs. 5, 36, 47, 87]

Unconventional composition and preparation of sulfide hydrotreating catalysts

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

The principles of the ZrO_2-CeO_2 support synthesis and impregnation of the carries Al_2O_3, ZrO_2, and SiO_2- Al_2O_3 with the use of complexing agents to deposit transition metals (Co, Ni, Mo, and selected platinum metals) and with the use of organic solvent solubility precursors e.g. metals acetylacetonates were studied to prepare highly active catalysts in model hydrodesulfurization of thiophene, benzothiophene, hydrodeoxygenation of rape-seed oil and isomerization of 1-methyl-cyclohex-1-ene. The synergism in the activities and the relative C-S hydrogenolysis/ C=C hydrogenation/C=C isomerization and triglycerides hydrogenolysis / triglycerides decarboxylation selectivities were determined. The original method of slurry impregnation (solvent-assisted spreading) was successfully modified for direct synthesis of the catalysts. [Refs. 5, 28, 48-51, 92]

Reactive chemical barriers for decontamination of heavily polluted waters

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

The project is focused on the practical development of special oxidation processes used for decontamination of industrially polluted subsurface waters. The used methods were: 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 were tested on a laboratory scale, in parallel they were modified and scaled-up for practical testing on three selected industrial sites. The efficiencies of the chosen methodologies were compared and the most suitable one were implemented to the final form. This system will be produced and long-term tested. [Refs. 9, 10, 24]

Composed molecular templates for preparation of assembled functional nanoparticles

(P. Klusoň, kluson@icpf.cas.cz; joint bilateral project with Bangor University, School of Chemistry, Wales, UK; supported by ASCR, 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 also scientific concepts. These attempts were reflected in the steep growth of interest in nanoscience and nanotechnologies. There was much progress in the synthesis, assembly and fabrication of nanomaterials. Similar 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. 8, 30, 31, 35, 56]

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

(O. Šolcová, solcova@icpf.cas.cz; joint project with Dekonta a.s.; supported by MIT, 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 the waste by thermal desorption process and subsequent catalytic oxidation of desorbed organic contaminants. Research activities aimed at solution of some technical problems related to full-scale application of the developed technology will be realized together with testing under real conditions. [Ref. 5]

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

(O. Šolcová, solcova@icpf.cas.cz; joint project with CU, supported by GACR, grant No. 204/11/1206)

Searching after the functional relationship between diffusion of fluid in disordered solids (e.g. porous solids) and their microstructure is an active field of research in membrane science, catalysis, biophysics, civil engineering and other branches of research and development. During several past decades the pulsed field gradient (PFG) NMR technique has proved to be a powerful tool for measuring of self-diffusion in such systems. The focus of the project will be on investigation of transport of liquid species contained in porous materials (non-consolidated and consolidated) with monodisperse and bidisperse porous structure with excursions to adjacent supercritical regions. A rational system of transport-related structure characteristics to predict transport behavior of liquids and supercritical fluids will be searched by combined application of PFG NMR, image analysis of porous materials and molecular simulation of self-diffusion in selected two-phase systems. [Refs. 22, 42, 82, 84]

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

(O. Šolcová, solcova@icpf.cas.cz; supported by TACR, grant No. 01020804)

The necessity to find alternative solutions for environmental protection leads to the development and use of the new technologies. Photo-catalysis using semiconductor oxides have found an increasing interest to solve the global pollution problems. Compared to the other photo-catalysts TiO_2 (and/or doped TiO_2) seems to be the most promising material not only in advanced oxidation photo-catalytic processes (AOP). It is well established that titanium oxide and related nanostructure materials in the presence of UV light (in dependence on conditions also in the presence of visible-light) can create very active species that are able to restore and preserve a clean environment by decomposing harmful organics; killing bacteria and viruses and being easily self-cleaned. Our investigation insists on the photo-catalyst immobilization in the form of a thin film trying to improve the efficiency of photocatalytic processes. [Refs. 42, 54, 55, 82, 84]

New heterogeneous catalysts for environmental protection

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

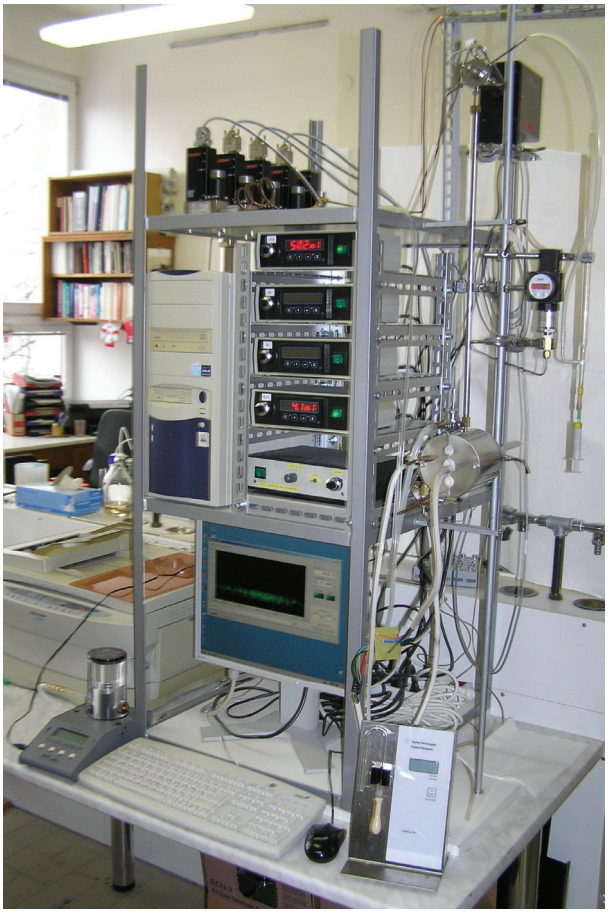
The hydrotreating NiMo/γ-Al_2O_3 catalyst (12 wt% Mo and 1.1 wt% Ni) has been prepared by impregnation of the support with the Anderson-type heteropolyoxomolybdate $(NH_4)_4[Ni(OH)_6Mo_6O_{18}]$. The modified catalysts have been synthesized by impregnation of the support with an aqueous solution of H_3BO_3, $Co(NO_3)_2$ or $Ni(NO_3)_2$ before the deposition of heteropolyoxomolybdate. The addition of Co, Ni, or B has influenced both the phase

composition and catalytic activity of the 1-benzothiophene hydrodesulfurization reaction. Preliminary loading of Ni, Co or B increased the sulfidity of the NiMo/γ-Al_2O_3 catalysts, which was confirmed by X-ray photoelectron micro-analysis. Nanoparticles of TiO_2-ZrO_2 mixtures and tungsten-modified SBA-15 and HMS were studied for hydrotreating reactions. Acid-base properties of K-promoted (K,Ni)Mo/Al_2O_3 catalyst and its activity in the sour water-gas shift were examined. [Refs. 3, 49, 50, 76]

Transport characteristics of novel biocompatible materials

(K. Soukup, soukup@icpf.cas.cz; supported by GACR, grant No. 106/11/P459)

The development and design of advanced bioactive and biocompatible porous materials for medical applications requires a thorough understanding of the texture and transport properties impact on their clinical efficiency. The proposed project will be focused on mass transport measurements and the transport characteristic determination of biocompatible clinical valuable materials consisted of apatite, hydroxyapatite and nanofiber membranes. Transport characteristics will be determined in liquid/solid as well as gas/solid systems by combination of inverse liquid chromatography and Graham's diffusion cell methods. Effective diffusion coefficients in liquid phase will be evaluated using a method based on the fitting of a set of experimental chromatographic profiles to the Kubín-Kučera model. Fitting of the gas diffusion data obtained from Graham's diffusion cell to the Mean Transport-Pore Model will provide transport characteristics. The obtained transport parameters will be compared with characteristics from standard textural analyses. [Refs. 81, 82, 84]



Inverse gas chromatography setup

International co-operations

University of Ghent, Ghent, Belgium: Theory of chemical bond, theoretical characterization of aromaticity
Institut Scientifique de Service Public, Liege, Belgium: Transport characteristics for coal gasification
University of Ghent, Ghent, Belgium: Generalized population analysis, theoretical characterization of aromaticity, molecular basis of structure activity relationships
Institute of Catalysis, BAS, Sofia, Bulgaria: New heterogeneous catalysts for environmental protection
University of Oulu, Oulu, Finland: New catalysts for VOC oxidation
University of Paris VI, Paris, France: Theory of chemical bond
University of Poitiers, Poitiers, France: New catalysts for VOC elimination
University of Strasbourg, Strasbourg, France: Determination of transport characteristics of novel materials with hierarchical pore structure
University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix
Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Visualization of bonding interactions in transition metal complexes
Department of Chemical Sciences, University of Padua, Padua, Italy: Polymer-based catalysts
Silesian University of Technology, Gliwice, Poland: Transport characteristics for coal gasification
Central Mining Institute, Katowice, Poland: Transport characteristics for coal gasification
University of Kragujevac, Serbia: Multicenter bonding, quantitative characterization of aromaticity
Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia: Morphology of Poly-HIPE materials
University of Vigo, Vigo, Spain: Multicenter bonding, theoretical characterization of aromaticity
Institute of Surface Chemistry NAS, Kiev, Ukraine: Preparation of nanoporous materials
University of Bangor, Bangor, Wales, United Kingdom: New sensors based on optically active nanomaterials
University of Liverpool, Liverpool, United Kingdom: Theory of chemical bond
UCG Partnership Ltd, Woking, United Kingdom: Transport characteristics for coal gasification
University of Udine, Udine, Italy: Characterization of noble metal catalysts and desulfurization on unconventional catalysts
Department of Physical chemistry, Slovak Technical University Bratislava, Slovakia: visualization of bonding interactions in transition metal complexes
Chemistry department, University of Pecs, Hungary: visualization of the bonding interactions in transition metal complexes

Visitors

M. Boltz, University of Strasbourg, France
L. Bučinský, Slovak Technical University Bratislava, Slovakia
P. Bultinck, Ghent university, Belgium
D. Cooper, University of Liverpool, United Kingdom

B. Corain, University of Padua, Italy
P. Krajnc, University of Maribor, Slovenia
P. G. Mezey, Memorial university of New Foundland, Canada
M. Mitoraj, Jagellonian university Krakow, Poland
S. Ojala, University of Oulu, Finland
S. Pitkäaho, University of Oulu, Finland
A. Spojakina, Institute of cataysis, BAS, Sofia, Bulgaria
Y. Zub, Institute of Surface Chemistry NAS, Ukraine

Teaching

P. Klusoň: UJEP, course "Toxicology"
R. Ponec: CU, course "Structure and reactivity"
O. Šolcová: ICT, postgraduate course "Texture of porous solids"

Publications

Original papers

[1] Čapek P., Hejtmánek V., Kolafa J., Brabec L.: Transport Properties of Stochastically Reconstructed Porous Media with Improved Pore Connectivity. *Transp. Porous Media* 88(1), 87-106 (2011).

[2] Černá I., Klusoň P., Bendová M., Floriš T., Pelantová H., Pekárek T.: Intensification of the Use of Ionic Liquids as Efficient Reaction Co-Solvents in Asymmetric Hydrogenations. *Chem. Eng.Process.* 50(3), 264-272 (2011).

[3] Dimitrov L., Palcheva R., Spojakina A., Jirátová K.: Synthesis and Characterization of W-SBA-15 and W-HMS as Supports for HDS. *J. Porous Mat.* 18(4), 425-434 (2011).

[4] Floriš T., Klusoň P., Slater M.: Stereoselective Hydrogenation of Methyl Acetoacetate over Structurally Different Chiral Ruthenium Complexes. *React. Kinet. Mech. Cat.* 102(1), 67-74 (2011).

[5] Gaálová J., Topka P., Kaluža L., Šolcová O.: Gold versus Platinum on Ceria-Zirconia Mixed Oxides in Oxidation of Ethanol and Toluene. *Catal. Today* 175(1), 231-237 (2011).

[6] Kaštánek P., Kaštánek F., Hájek M., Sobek J., Šolcová O.: Dehalogenation of Polychlorinated Biphenyls (PCB) by Nucleofile Reactants at the Presence of Ionic Liquids and under Application of Microwaves. *Global NEST J.* 13(1), 59-64 (2011).

[7] Kegl T., Ponec R., Kollar L.: Theoretical Insights into the Nature of Nickel-Carbon Dioxide Interactions in $Ni(PH_3)_2(\eta^2\text{-}CO_2)$. *J. Phys. Chem. A* 115(45), 12463-12473 (2011).

[8] Klusoň P., Krýsa J., Malato S., Oller I.: Selected Contributions of the 6th European Meeting on Solar Chemistry and Photocatalysis: Environmental Applications (SPEA 6), 13-16 June 2010, Introduction. *Catal. Today* 161(1), 2 (2011).

[9] Klusoň P., Hejda S., Hejdová M, Krýsa J: A Genuine Way to Mimic the Solar-Light Conditions in UV Driven Heterogeneous Photocatalytic Reactions. *Reac. Kinet. Mech. Cat.* 104(2), 273-280 (2011).

[10] Klusoň P., Hejda S., Koudleková L., Hejdová M., Krýsa J.: Je možné objektivně srovnávat aktivitu heterogenních fotokatalytických reakcí? (Czech) Is it Possible to Compare Objectively Activities of Heterogeneous Photocatalysts in a Liquid Phase? *Chem. Listy* 105(10), 738-744 (2011).

[11] Kment S., Hubička Z., Kmentová H., Klusoň P., Krýsa J., Gregora I., Morozová M., Čada M., Petráš D., Dytrych P., Slater M., Jastrabík L.: Photoelectrochemical Properties of Hierarchical Nanocomposite Structure: Carbon Nanofibers/TiO_2/ZnO Thin Films. *Catal. Today* 161(1), 8-14 (2011).

[12] Kočí K., Zatloukalová K., Obalová L., Krejčíková S., Lacný Z., Čapek L., Hospodková A., Šolcová O.: Wavelength Effect on Photocatalytic Reduction of CO_2 by Ag/TiO_2 Catalyst. *Chin. J. Catal.* 32(5SI), 812-815 (2011).

[13] Kovačič S., Jeřábek K., Krajnc P.: Responsive Poly(acrylic acid) and Poly(N-isopropyl-acrylamide) Monoliths by High Internal Phase Emulsion (HIPE) Templating. *Macromol. Chem. Phys.* 212(19), 2151-2158 (2011).

[14] Kovanda F., Jirátová K.: Supported Layered Double Hydroxide-Related Mixed Oxides and Their Application in the Total Oxidation of Volatile Organic Compounds. *Appl. Clay Sci.* 53(2), 305-316 (2011).

[15] Kovanda F., Jirátová K.: Supported Mixed Oxide Catalysts for the Total Oxidation of Volatile Organic Compounds. *Catal. Today* 176(1), 110-115 (2011).

[16] Matěj Z., Matějová L., Novotný F., Drahokoupil J., Kužel R.: Determination of Crystallite Size Distribution Histogram in Nanocrystalline Anatase Powders by XRD. *Z. Kristallogr. Proc.* 1, 87-92 (2011).

[17] Morozová M., Klusoň P., Krýsa J., Dzik P., Veselý M., Šolcová O.: Thin TiO_2 Films Prepared by Inkjet Printing of the Reverse Micelles Sol-Gel Composition. *Sens. Actuator B-Chem.* 160(1), 371-378 (2011).

[18] Morozová M., Klusoň P., Krýsa J., Gwenin Ch., Šolcová O.: Oxalic Acid Sensors Based on Sol-Gel Nanostructured TiO_2 Films. *J. Sol-Gel Sci. Technol.* 58(1), 175-181 (2011).

[19] Obalová L., Jirátová K., Karásková K., Kovanda F.: Simulation of N_2O Abatement in Waste Gases by Its Decomposition over a K-Promoted Co-Mn-Al Mixed Oxide Catalyst. *Chin. J. Catal.* 32(5(SI)), 816-820 (2011).

[20] Ojala S., Pitkäaho S., Laitinen T., Koivikko N.N., Brahmi R., Gaálová J., Matějová L., Kucherov A., Päivärinta S., Hirschmann C., Nevanperä T., Riihimäki M., Pirilä M., Keiski R.L.: Catalysis in VOC Abatement. *Top. Catal.* 54(16-18), 1224-1256 (2011).

[21] Ponec R.: Bond Indices in Solids: Extended Analytical Model. *J. Comput. Chem.* 32(14), 3114-3121 (2011).

[22] Salejová G., Grof Z., Šolcová O., Schneider P., Kosek J.: Strategy for Predicting Effective Transport Properties of Complex Porous Structures. *Comput. Chem. Eng.* 35(2), 200-211 (2011).

[23] Soukup K., Rogut J., Grabowski J., Wiatowski M., Ludwik-Pardała M., Schneider P., Šolcová O.: Preparation and Microstructure Characterization of Iron Oxide Pellets for Hydrogen Storage. *Int. J. Systems Applications, Engineering & Development* 5(3), 334-341 (2011).

[24] Šolcová O., Klusoň P., Soukup K., Krystyník P., Wimmerová L.: Texturní a transportní charakteristiky půdních vzorků v areálu bývalého chemického výrobního závodu Deza Ostrava. (Czech) Textural and Transport Characteristics of the Soil Samples from the Area of the Former Chemical Production Plant Deza Ostrava. *Waste Forum* 4(1), 42-49 (2011).

[25] Šolcová O., Matějová L., Topka P., Musilová Z., Schneider P.: Comparison of Textural Information from Argon (87 K) and Nitrogen (77 K) Physisorption. *J. Porous Mat.* 18(5), 557-565 (2011).

[26] Topka P., Karban J., Soukup K., Jirátová K., Šolcová O.: Preparation of Al-SBA-15 Pellets with Low Amount of Additives: Effect of Binder Content on Texture and Mechanical Properties. Application to Friedel-Crafts Alkylation. *Chem. Eng. J.* 168(1), 433-440 (2011).

[27] Vít Z., Kaluža L., Gulková D.: Nitrogen Tolerant Hydrodesulfurization Catalysts Based on Rh and Ru Promoted Mo/Al_2O_3. *Top. Catal.* 54(16-18), 1325-1330 (2011).

[28] Vít Z., Kmentová H., Kaluža L., Gulková D., Boaro M.: Effect of Preparation of Pd and Pd-Pt Catalysts from Acid Leached Silica-Alumina on Their Activity in HDS of Thiophene and Benzothiophene. *Appl. Catal., B* 108(1-2), 152-160 (2011).

Patents

[29] Jeřábek K., Hanková L., Holub L., Corain B., Zecca M., Centomo P., Bonato I.: Silně kyselý ionexový katalyzátor s afinitou k lipofilním reagentům a způsob jeho přípravy. (Czech) Strongly Acidic Ion Exchanger Catalysts Having Affinity towards Lipophilic Reagents and Method of Its Preparation. Pat. No. *PV2011-146*. Applied: 11.03.22.

International conferences

[30] Baranov A.I., Kohout M., Ponec R.: Domain Averaged Fermi hole Orbitals for Extended Systems. Prague Workshop on Theoretical Chemistry, Book of Abstracts, p. 7-8, Praha, Czech Republic, 26-29 September 2011.

[31] Barcs B., Kollár L., Ponec R., Kégl T.: Electronic Structure of Ni(0) Complexes Containing Ligands with Cumulative Double Bonds. Prague Workshop on Theoretical Chemistry, Book of Abstracts, p. 28-30, Praha, Czech Republic, 26-29 September 2011.

[32] Centomo P., Bonato I., Hanková L., Holub L., Jeřábek K., Zecca M.: Ion Exchanger Catalyst Modification for Reactions Involving Lipophilic Reagents. XXIV Congresso Nazionale della Società Chimica Italiana, Atti del Congresso, p. 607, Lecce, Italy, 11-16 September 2011.

[33] Čapek L., Smoláková L., Priecel P., Kutálek P., Hájek M., Bulánek R., Kubičková I., Matějová L.: Analysis of Basic Sites at Solid-Base Catalysts. 4th International Symposium Advanced Micro- and Mesoporous Materials 2011, Book of Abstracts, p. 110, Riviera Resort, Bulgaria, 6-9 September 2011.

[34] Čapek P., Veselý V., Kolafa J., Hejtmánek V., Brabec L.: Simulace transportu hmoty v replikách pórovitých látek pro účely odhadu jejich efektivních transportních vlastností. (Czech) Mass Transport Simulation in Replicas of Porous Material: Effective Transport Properties Estimation. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 25 (B1.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[35] Dytrych P., Klusoň P., Floriš T., Lísal M., Slater M.: Theoretical Interpretation of Enantioselectivity Trends in (*R*)-Ru-BINAP Catalyzed Hydrogenation of Methylacetoacetate in the QAS Ionic Liquid Phase. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 35 (C1.5), Srní, Šumava, Czech Republic, 24-27 October 2011.

[36] Gaálová J., Kaluža L., Topka P.: New Catalysts for VOC Oxidation Based on Ce-Zr Mixed Oxides. 25th National Chemistry Congress, Abstracts Book for Poster Presentations, p. 208 (OP-183), Ankara, Turkey, 27 June - 2 July 2011.

[37] Gaálová J., Kaluža L., Topka P., Matějová L.: Total Oxidation of Ethanol and Dichloromethane over Ceria-Zirconia Mixed Oxides Doped with Platinum and Gold. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1302-1303, Tatranské Matliare, Slovakia, 23-27 May 2011.

[38] Gulková D., Vít Z.: Inhibitive Effect of Pyridine and Toluene on HDS of Thiophene over Mo/Al_2O_3 Based Catalysts. 43. Symposium on Catalysis, Program Book of Abstracts, P06A, Prague, Czech Republic, 7-8 November 2011.

[39] Gulková D., Vít Z., Kaluža L., Kmentová H., Zdražil M., Boaro M.: Activity of Pd and Mo HDS Catalysts Supported on Modified Silica-Alumina. 8th European Congress of Chemical Engineering, P 19.06, Berlin, Germany, 25-29 September 2011.

[40] Hanková L., Holub L., Jeřábek K.: Ion Exchanger Catalyst Modification for Reactions Involving Lipophilic Reagents. 38th International Conference of Slovak Society of Chemical Engineering , Proceedings, p. 1190-1192, Tatranské Matliare, Slovakia, 23-27 May 2011.

[41] Hanková L., Jeřábek K.: Modeling of Swollen State Morphology of Functional Polymers. 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 031, Santiago de Compostella, Spain, 17-22 July 2011.

[42] Hejtmánek V., Čapek P.: 3D Microstructure Modelling of Real Porous Steel Material from 2D Images. 7th International Conference on Porous Metals and Metallic Foams MetFoam2011, Abstracts Book, p. 269, Busan, South Korea, 18-21 September 2011.

[43] Jeřábek K., Holub L., Hanková L., Corain B., Centomo P.: Adsorption Assisted Ion Exchanger Catalyst for Fatty Acid Esterification. 19th IUPAC International Conference on Chemical Research Applied to World Needs (CHEMRAWN XIX) 2011, Programme and Abstracts, p. 18, Kuala Lumpur, Malaysia, 27-29 September 2011.

[44] Jeřábek K., Holub L., Hanková L., Corain B., Centomo P., Zecca M.: Adsorption Assisted Ion Exchanger Catalyst for Fatty Acid Esterification. 43th Symposium on Catalysis, Book of Abstracts, OP14, Praha, Czech Republic, 7-8 November 2011.

[45] Jirátová K., Kovanda F.: Total Oxidation of Toluene over Calcined Layered Double Hydroxides Containing Various Transition Metals. European Clay Conference EUROCLAY 2011, Book of Abstracts, p. 345, Antalya, Turkey, 26 June - 1 July 2011.

[46] Jirátová K., Mikulová Z., Klempa J., Kovanda F.: Modificarion of Calcined Ni-Mg-Mn and Co-Mn-Al LDHs with Platinum: Properties and Activity in Total Oxidation of VOC. Europacat X, PM111, Glasgow, Great Britain, 29 August - 2 September 2011.

[47] Kaluža L., Gaálová J., Topka P., Matějová L., Gulková D.: Total Oxidation of Model Volatile Organic Compounds over Ceria-Zirconia Mixed Oxides Doped with Platinum and Gold. 8th European Congress of Chemical Engineering, P05.01, Berlin, Germany, 25-29 September 2011.

[48] Kaluža L., Kubička D.: Hydrodeoxygenation of Rapeseed Oil over Sulfided Ni, Mo and NiMo Catalysts. 8th European Congress of Chemical Engineering, P20.01, Berlin, Germany, 25-29 September 2011.

[49] Kaluža L., Palcheva R., Spojakina A., Jirátová K., Tyuliev G.: Hydrodesulfurization Activity of Alumina Supported Anderson Heteropolymolybdates Doped with Co, Ni and B. Europacat X, Posters, PT63, Glasgow, Great Britain, 29 August - 2 September 2011.

[50] Kaluža L., Palcheva R., Spojakina A., Jirátová K., Tyuliev G.: Alumina Modified with Co, Ni and B as a Support of Hydrodesulfurization Catalysts Prepared from Anderson Heteropolymolybdates. 43th Symposium on Catalysis, Book of Abstracts, P12A, Prague, Czech Republic, 7-8 November 2011.

[51] Kaluža L., Sýkora J., Karban J., Žáček P., Vít Z., Zdražil M.: Hydrodesulfurization of Model Feed Containing Olefins over Al_2O_3, TiO_2, and ZrO_2 Supported Transition Metal Sulfides. 8th European Congress of Chemical Engineering, Programme, P19.01, Berlin, Germany, 25-29 September 2011.

[52] Karásková K., Chromčáková Ž., Študentová S., Obalová L., Jirátová K.: Co-Mn-Al Mixed Oxide Supported on TiO_2 for N_2O Decomposition. International Symposium on Nitrogen Oxides Emission Abatement, Book of Abstracts, p. 155, Zakopane, Poland, 4-7 September 2011.

[53] Karásková K., Kulová T., Obalová L., Jirátová K., Kovanda F.: Alkali Metals Promoted Co-Mn-Al Mixed Oxide for N_2O Catalytic Decomposition. 38th International Conference of Slovak Society of Chemical Engineering , Proceedings, p. 1304-1309, Tatranské Matliare, Slovakia, 23-27 May 2011.

[54] Kaštánek F.: Biotechnologie pro chemický průmysl. (Czech) Biotechnology for Chemical Industry. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 99 (C4.1), Srní, Šumava, Czech Republic, 24-27 October 2011.

[55] Kaštánek F., Sobek J., Kaštánek P., Šolcová O., Hájek M.: Dehalogenation of Polyhalogenated Compounds Dissolved in Organic Solvents with the Help of AOPs in a Two-Phase Solvent-Water System under the Influence of Ultrasound. 12th International Conference on Environmental Science and Technology CEST 2011, Proceedings, p. 114, Dodecanese, Rhodes Island, Greece, 8-10 September 2011.

[56] Klusoň P., Hejda S.: Critical Notes on Heterogeneous Photocatalysis on TiO_2 Photocatalysts. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 52 (C2.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[57] Kočí K., Krejčíková S., Lacný Z., Šolcová O., Obalová L.: Photocatalytic Decomposition of N_2O on Ag-TiO_2. International Symposium on Nitrogen Oxides Emission Abatement, Book of Abstracts, pp. 159-161, Zakopane, Poland, 4-7 September 2011.

[58] Krejčíková S., Kočí K., Obalová L., Čapek L., Šolcová O.: Optimized Doped Titania for Photocatalysis Applications. 2nd Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 54 (PP-6), Ostrava, Czech Republic, 27-29 April 2011.

[59] Krejčíková S., Maléterová Y., Matěj Z., Šolcová O.: Preparation and Characterization of Doped Titania Layers for Polluted Water Cleaning. 9th International Symposium on the Characterisation of Porous Solids - COPS 9, Book of Abstracts, p. 78, Dresden, Germany, 5-8 June 2011.

[60] Krejčíková S., Maléterová Y., Šnajdaufová H., Šolcová O.: Doped Titania Photocatalysts for Poluted Water Cleaning; Preparation and Characterization. 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 031, Santiago de Compostela, Spain, 17-22 July 2011.

[61] Ludvíková J., Jirátová K., Klempa J.: Titania Supported Co-Mn-Al Catalysts in Total Oxidation of Ethanol. 4th Czech-Italian-Spanish Symposium on Molecular Sieves and Catalysis, Book of Abstracts, O21, Liblice, Czech Republic, 15-18 June 2011.

[62] Ludvíková J., Jirátová K., Kovanda F.: Mixed Oxides of Transition Metals as Catalysts for Total Ethanol Oxidation. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 231, Tatranské Matliare, Slovakia, 23-27 May 2011.

[63] Ludvíková J., Jirátová K., Kovanda F., Klempa J.: Úplná oxidace organických látek obsažených ve vzduchu na oxidických katalyzátorech. (Czech) Total Oxidation of Organic Compounds in Air over Oxide Catalysts. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, pp. 692-697, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

[64] Maléterová Y., Krejčíková S., Šnajdaufová H., Cajthaml T., Šolcová O.: Comparison of Various Titania Photocatalysts by the Contaminated Water Cleaning. 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 032, Santiago de Compostella, Spain, 17-22 July 2011.

[65] Matějová L., Fajgar R., Matěj Z., Maléterová Y., Šolcová O.: Metal Oxide Aerogel. 2nd Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 11(OP-5), Ostrava, Czech Republic, 27-29 April 2011.

[66] Matějová L., Matěj Z., Fajgar R., Schneider P., Šolcová O.: Highly-Porous Metal Oxide Aerogels; Preparation and Characterization. 9th International Symposium on Characterization of Porous Solids - COPS 9, Book of Abstracts, p. 181, Dresden, Germany, 5-8 June 2011.

[67] Matějová L., Matěj Z., Fajgar R., Šolcová O.: Role of Subcritical Water Extraction in Crystallization of Highly-Porous Titania, Titania-Zirconia and Titania-Ceria Aerogels. 12th Conference of the European Ceramic Society ECerS XII, Poster Session II, p. 72 (2132), Stockholm, Sweden, 19-23 June 2011.

[68] Matějová L., Matěj Z., Fajgar R., Šolcová O.: Role of Subcritical Drying in Preparation of Crystalline Metal Oxides Aerogels. 4th International Symposium Advanced Micro- and Mesoporous Materials 2011, Book of Abstracts, p. 72, Riviera Resort, Bulgaria, 6-9 September 2011.

[69] Matějová L., Šnajdaufová H,, Matějková M., Fajgar R., Matěj Z., Šolcová O.: Optimization of Pressurized Fluid Extraction for Preparation of Metal Oxide Nanostructures. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, pp. 1207-1210, Tatranské Matliare, Slovakia, 23-27 May 2011.

[70] Morozová M., Klusoň P., Dzik P., Veselý M., Krýsa J., Šolcová O.: Thin Sol-Gel TiO_2 Films Prepared by Inkjet Printing – Photoelectrochemical Properties. 4th Czech-Austrian Workshop: New Trends in Photo- and Electro- Catalysis, Hnanice, Czech Republic, 5-7 December 2011.

[71] Morozová M., Klusoň P., Hejda S., Kment Š., Šolcová O.: Thin Functional Films of TiO_2 Nanoparticles. 44th Heyrovský Discussion - Nanostructures on Electrodes, Book of Abstracts, p. 56, Třešť, Czech Republic, 26-30 June 2011.

[72] Morozová M., Klusoň P., Krýsa J., Veselý V., Dzik P., Šolcová O.: Thin TiO_2 Sol-gel Layers Deposited by Three Various Methods. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, pp. 1211-1213, Tatranské Matliare, Slovakia, 23-27 May 2011.

[73] Morozová M., Klusoň P., Veselý M., Dzik P., Šolcová O.: The Ink-Jet Printed Nanostructured TiO_2 Film Electrode. 2nd Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 12 (OP-6), Ostrava, Czech Republic, 27-29 April 2011.

[74] Morozová M., Klusoň P., Veselý M., Dzik P., Šolcová O.: Photo-Electrochemistry on the Thin TiO_2 Sol-Gel Layers Deposited by Ink-Jet Printing. 12th Conference of the European Ceramic Society ECerS XII, Poster Session II, p. 72 (2133), Stockholm, Sweden, 19-23 June 2011.

[75] Morozová M., Klusoň P., Veselý M., Dzik P., Šolcová O.: Photo-Electrochemical Characterization of Thin TiO_2 Sol-Gel Layers Deposited by Dip-Coating and Injekt Printing. 9th International Symposium on the Characterisation of Porous Solids - COPS 9, Book of Abstracts, p. 99, Dresden, Germany, 5-8 June 2011.

[76] Nikolova D., Edreva-Kardjieva R., Spojakina A., Jirátová K.: Potassium Influence on Acid-Base Properties of the Sour Water-Gas Shift (K,Ni)Mo/γ-Al_2O_3 Catalysts. Europacat X, Posters, PM271, Glasgow, Great Britain, 29 August - 02 September 2011.

[77] Obalová L., Jirátová K., Kovanda F.: NO_2 Catalytic Decomposition - from Laboratory Experiment to Industry Reactor. International Symposium on Nitrogen Oxides Emission Abatement, Book of Abstracts, p. 97, Zakopane, Poland, 04-07 September 2011.

[78] Ponec R., Cooper D.L.: Splitting and/or Formation of Chemical Bonds. Insights from Momentum Space. 4th JCS Symposium on Theoretical Chemistry 2011, Conference Book, p. 1, Liblice, Czech Republic, 18-20 May 2011.

[79] Ponec R., Kohout M.: Bond Indices in Solids. A Numerical Approach to Analytical Model. Prague Workshop on Theoretical Chemistry, Book of Abstracts, pp. 44-50, p. 7, Praha, Czech Republic, 26-29 September 2011.

[80] Ponec R., Salvador P., Ramos-Córdoba E.: Bonding Quandary in Cu_3S_2 Core. Insights from the Analysis of Domain Averaged Fermi holes and the Analysis of the Local Spin. 9th Triennial Congress of the World Association of Theoretical and Computational Chemists, Posters, PI 037, Santiago de Compostella, Spain, 17-22 July 2011.

[81] Soukup K., Klusoň P., Šolcová O.: Electrospun Polymer Nanofibers-Gas Transport Measurements in Graham's Diffusion Cell. 8th European Congress of Chemical Engineering, Programme, P05.08, Berlin, Germany, 25-29 September 2011.

[82] Soukup K., Petráš D., Topka P., Slobodian P., Šolcová O.: Preparation and Characterization of Electrospun Poly(p-phenylene oxide) Membranes. 10th International Conference on Catalysis in Membrane Reactors, Book of Abstracts, pp. 210-211, Saint-Petersburg, Russia, 20-24 June 2011.

[83] Soukup K., Stanczyk K., Rogut J., Schneider P., Šolcová O.: Effect of Process Parameters on the Mass Transport Phenomena during Underground Coal Gasification. 4th International Conference GeoProc2011: Cross Boundaries Through THMC Integration, Conference Program, GP036, (6 pp. full text on CD-ROM), Perth, Australia, 6-9 July 2011.

[84] Soukup K., Topka P., Petráš D., Šolcová O.: Transportní a katalytické vlastnosti polymerních nanovlákenných vrstev připravených technikou elektrostatického zvlákňování. (Czech) Transport and Catalytic Properties of Polymeric Nanofibrous Layers Prepared by Electrospinning. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 53 (C2.3), Srní, Šumava, Czech Republic, 24-27 October 2011.

[85] Šolcová O., Cajthaml T., Krejčíková S., Kaštánek F., Maléterová Y.: Application of Titania Thin Layers for Contaminated Water Cleaning. 9th International Symposium on the Characterisation of Porous Solids - COPS 9, Book of Abstracts, p. 84, Dresden, Germany, 5-8 June 2011.

[86] Šolcová O., Maléterová Y., Šnajdaufová H., Krejčíková S.: Thorough Characterization of Prepared TiO_2 - ZrO_2 Mixed Oxides for Photocatalytic Oxidation. 9th Triennial Congress of the World Association of Theoretical and Computational Chemists WATOC 2011, Posters, PII 035, Santiago de Compostella, Spain, 17-22 July 2011.

[87] Topka P., Kaluža L., Gaálová J.: Total Oxidation of Ethanol and Toluene over Platinum and Gold Supported on Ceria-Zirconia Mixed Oxide. 6th Asia Pacific Chemical Reaction Engineering Symposium, Abstract Coll., p. 127, Beijing, China, 18-21 September 2011.

[88] Vajglová Z., Vychodilová H., Kotas P., Kaštánek F., Jiřičný V.: Degradace polybromovaných difenyl éterů. (Czech) Degradation of Polybrominated Diphenyl Ethers. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, pp. 698-704, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

[89] Vajglová Z., Vychodilová H., Tříska J., Kaštánek F., Jiřičný V.: Degradation Methods for Polybrominated Diphenyl Ethers in Liquid Wastes. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 141-145, Tatranské Matliare, Slovakia, 23-27 May 2011.

[90] Vajglová Z., Vychodilová H., Křišťál J., Kaštánek F., Jiřičný V.: Selected Methods of Dehalogenation of Polybrominated Diphenyl Ethers. 8th European Congress of Chemical Engineering, Programme, P05.04, Berlin, Germany, 25-29 September 2011.

[91] Vít Z., Kmentová H., Gulková D., Kaluža L.: Mesoporous Silica-Alumina Modified by Acid Extraction as Support of Pd and Pd-Pt Catalysts in HDS of Model Compounds. 43th Symposium on Catalysis, Program and Book of Abstracts, P16B, Prague, Czech Republic, 7-8 November 2011.

[92] Vít Z., Kmentová H., Gulková D., Kaluža L.: Mesoporous Silica-Alumina Modified by Acid Extraction as Support of Pd and Pd-Pt Catalysts in HDS of Model Compounds. Europacat X, Posters, PT28, Glasgow, Great Britain, 29 August - 2 September 2011.

Department of Multiphase Reactors

HEAD
MAREK RŮŽIČKA

DEPUTY
PETR STANOVSKÝ

RESEARCH STAFF
JIŘÍ DRAHOŠ, MARIE FIALOVÁ, JAROMÍR HAVLICA, SANDRA KORDAČ ORVALHO, VĚRA PĚNKAVOVÁ, VÁCLAV SOBOLÍK, MIROSLAV ŠIMČÍK, JAROSLAV TIHON, VALENTIN TOVCHIGRECHKO, JIŘÍ VEJRAŽKA, ONDŘEJ WEIN, MÁRIA ZEDNÍKOVÁ

PHD STUDENTS
MARTIN BASZCZYŇSKI, LUKÁŠ KULAVIAK, PAVEL NOVÁK, LUCIE VOBECKÁ

TECHNICAL STAFF
STANISLAVA NOVÁKOVÁ

Fields of research

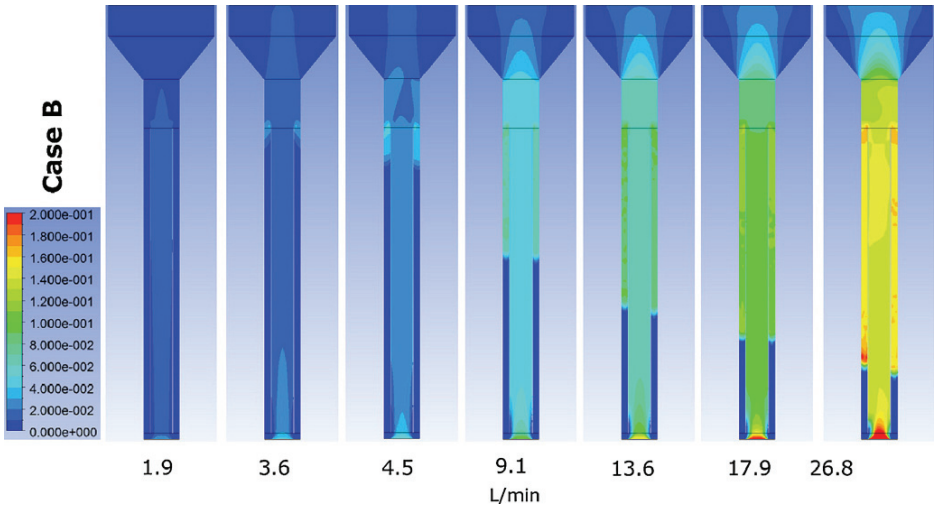
- Multiphase fluid dynamics and transport phenomena in different types of gas-liquid, liquid-solid or gas-liquid-solid systems
- Transport and reaction processes in complex multiphase systems
- Influence of surface active agents on the multiphase flows
- Flow of microdispersions and liquids with complex rheological behaviour
- Electrodiffusion diagnostics of the flow
- Flow characterization in T-shaped and cross-shaped micromixers
- Hydrodynamic concept of stromatactis formation in geology
- Determination of the coalescence efficiency of bubbles in liquids
- Dynamics of bubble formation at submerged orifices: Simultaneous formation and synchronous regimes
- Stability and behaviour of complex beverage foams

Research projects

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

(M. Růžička, ruzicka@icpf.cas.cz; joint project with TU of Ostrava; supported by GACR, grant No. 104/07/1110)

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. 5, 6, 10-12, 15, 18-22, 24]

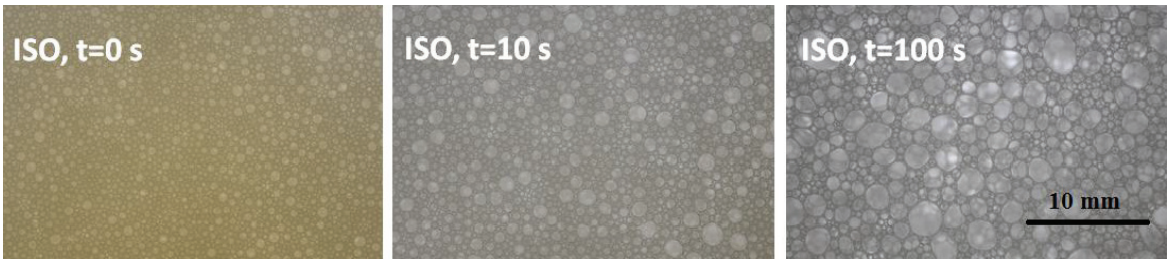


Local gas holdup (volume fraction of gas phase) in airlift for various gas flow rates on entrance

Transport and reaction processes in complex multiphase systems

(J. Drahoš, drahos@icpf.cas.cz; joint project with ICT and UPa; supported by GACR, grant No. 104/08/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 UPa, and at ICPF. Particular research programmes involve 16 areas from microsystems to industry-scale processes. Project is led by 18 supervisors. 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. 9, 13, 14, 29-33]

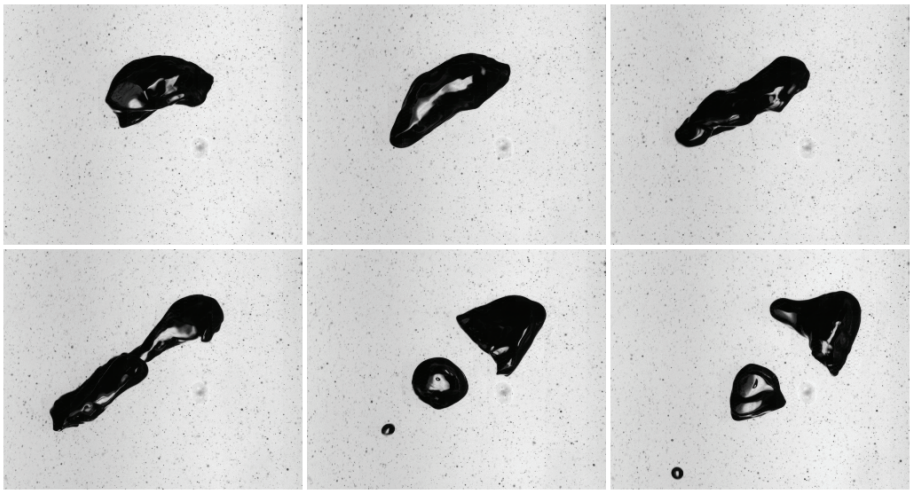


Structural changes in model beer foam with addition of a natural stabilisator (hop Iso-α-Acids)

Effect of surface-active agents on two-phase flows

(J. Vejražka, vejrazka@icpf.cas.cz; supported by GACR, grant No. 101/11/0806)

The effect of surface-active agents on two-phase flows is studied. Flow types "air bubbles in the liquid" and "liquid drops in another immiscible liquid" are focused. Some specific situations, in which the surfactants modify the flow at the bubble/drop scale and in which this modification cannot be explained by a simple change of the equilibrium surface tension, are investigated experimentally. These situations are (i) the shape oscillations of a bubble/drop, both freely-rising or attached at a capillary tip; focus is put on the modification of oscillation frequency and decay time by surfactants; (ii) the coalescence of bubbles/drops, and also their attachment to a solid surface, with a focus on the drainage of liquid film between them; (iii) the bubble-solid surface collision, with a focus on suppression of the bubble rebound caused by surfactants and also on the modification of the attachment time; (iv) break-up of bubbles in a turbulent flow. The research should enlighten and document the effect of interfacial properties other than surface tension on two-phase flows. [Refs. 8, 28-32]

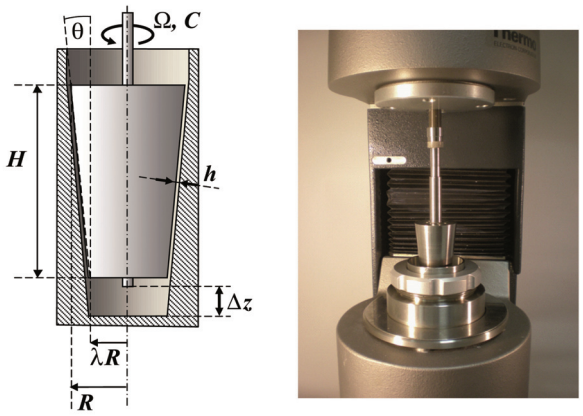


Break-up of a 5 mm bubble in a turbulent flow (interval between frames 12 ms)

Wall effect in flowing microdisperse liquids: apparent slip and electrokinetical potential

(O. Wein, wein@icpf.cas.cz; 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, 7, 16, 25-27, 33-35]

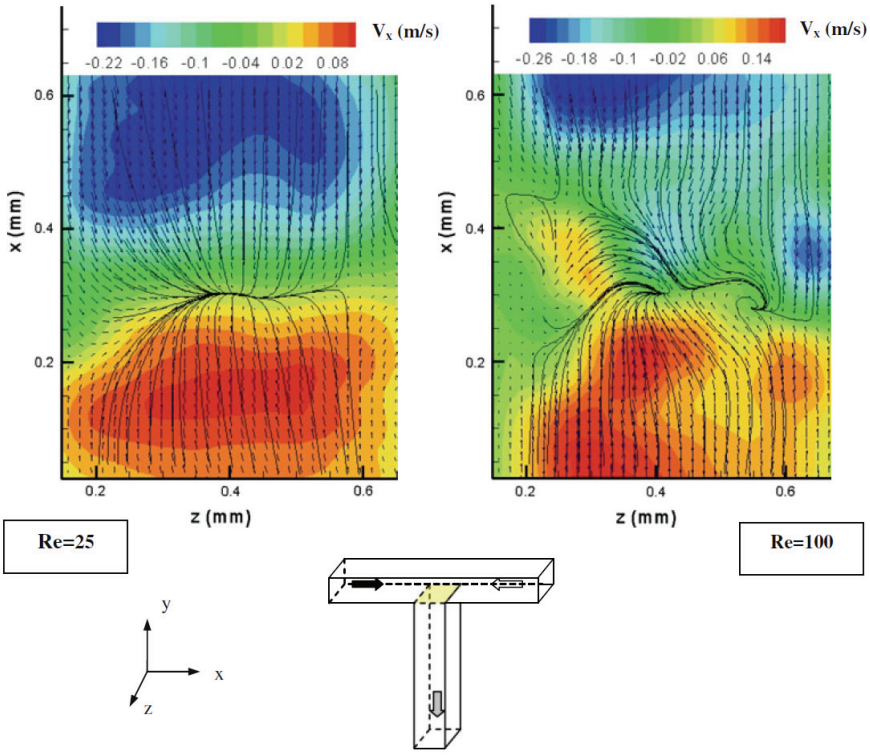


Original KK sensor for AWS viscometry

Flow characterization in T-shaped and cross-shaped micromixers

(J. Havlica, J. Tihon, havlica@icpf.cas.cz, tihon@icpf.cas.cz; joint project with GEPEA UMR-CNRS, Ecole des Mines de Nantes and University of Nantes, Saint-Nazaire, France;
supported by)

The understanding of physical phenomena such as flow behavior and mass transfer performance is needed in order to develop appropriate micromixers for industrial or biomedical applications. In this article, the flow behavior of the T-shaped and the cross-shaped micromixers with square cross-section are studied through numerical and experimental investigations. For experimental measurements of flow characterization were used particle image velocimetry (PIV) and electrodiffusion method. Results indicate that the cross-shaped micromixer could improve the mixing process in comparison with the micromixers having T geometry. [Refs. 1, 4, 23]

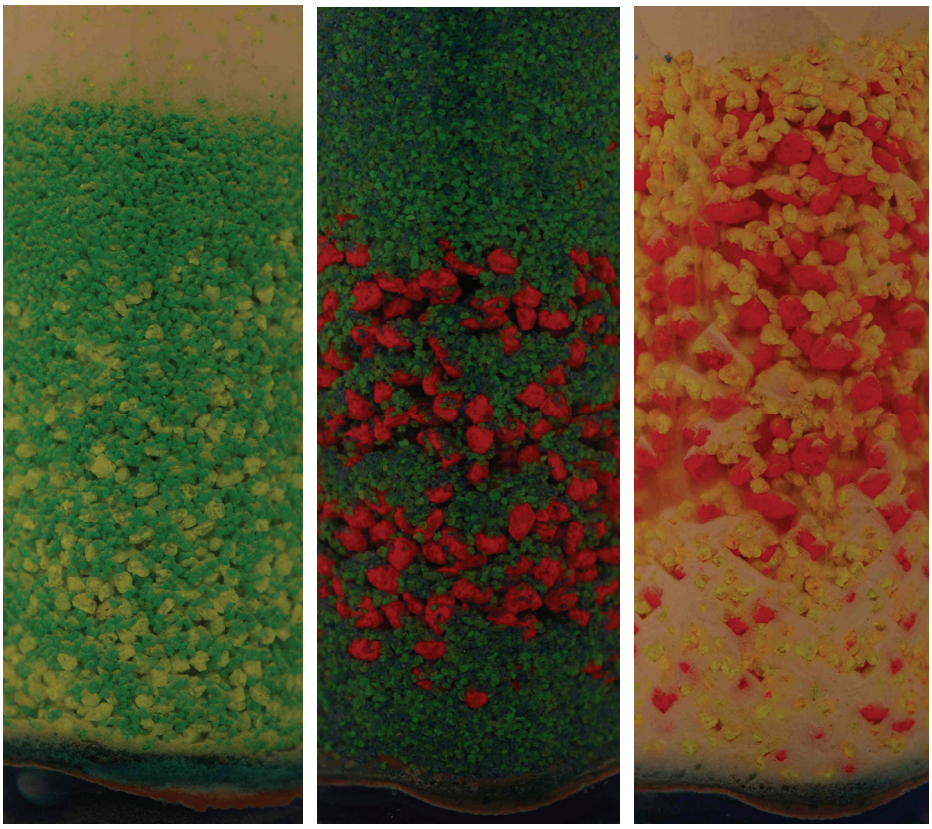


Velocity fields, streamlines and velocity profiles v_x in T-shaped micromixer for Re = 25 and Re = 100

Hydrodynamic concept of stromatactis formation in geology

(M. Růžička, ruzicka@icpf.cas.cz; joint project with Institute of Geology of the ASCR, v. v. i., supported by GA ASCR, 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 interdisciplinary study is novel, and the results are fundamental for sedimentology and hydrodynamics, with possible implications in related technologies. [Refs. 11, 12]

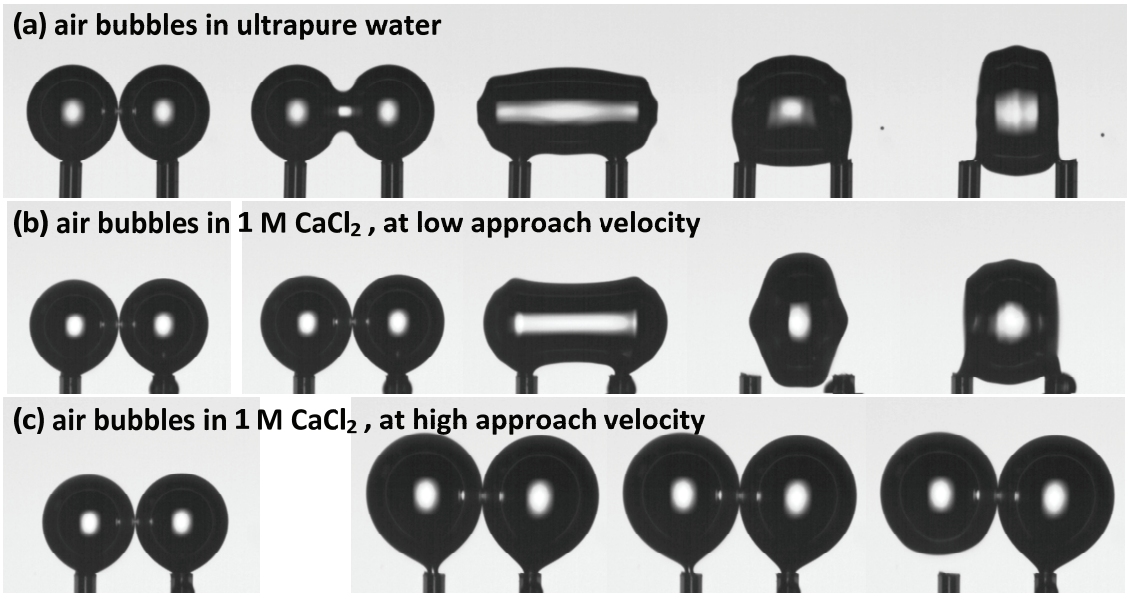


Effect of the missing fraction in five-fraction system on the formation of cavities

Determination of the coalescence efficiency of bubbles in liquids

(S. Kordač Orvalho, orvalho@icpf.cas.cz; supported by GACR, grant No. 104/09/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 and 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. 10, 15]

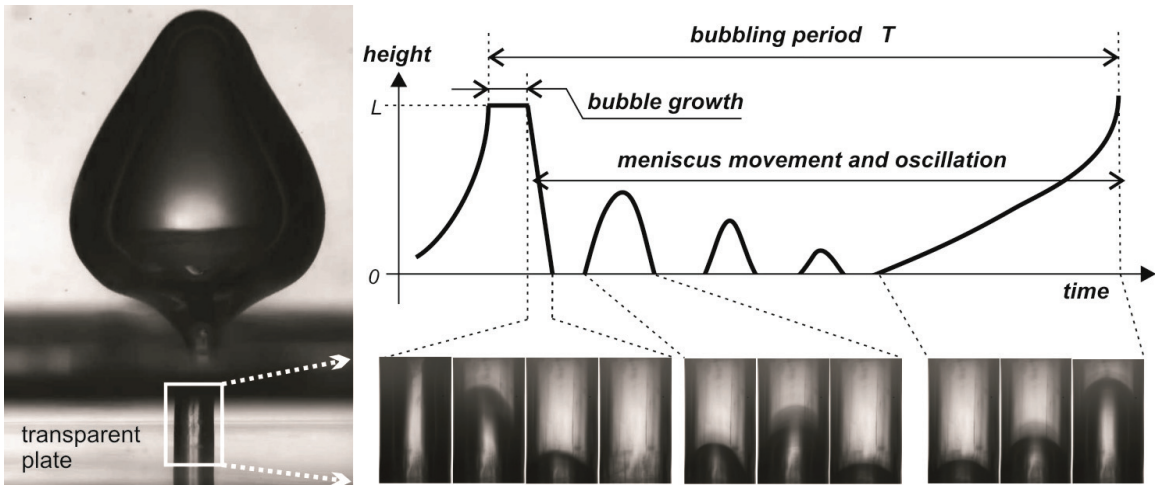


Effect of the approach velocity on the coalescence of air bubbles in coalescent ultrapure water and in non-coalescent calcium chloride, c(CaCl2) = 0.056 M

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

(P. Stanovský, stanovsky@icpf.cas.cz; supported by ASCR, grant No. KJB200720901)

Aim 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 two orifices together recorded with 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. 5, 18-20]



Meniscus oscillation influencing the bubble size variability and formation synchronicity

Presidency of the European Federation of Chemical Engineering (EFCE)
(J. Drahoš, drahos@icpf.cas.cz; supported by MEYS, INGO II, project No. LA11014)

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 and he continue its work as the member of Executive board. Together with Prof. Růžička, he also participates at the activities of the EFCE Working Party Multiphase Fluid Flow.

International co-operations

Berlin Institute of Technology, Germany: Multiphase flow diagnostics
CRTT, Saint Nazaire, France: Microfluidics
Institute of Fluid Mechanics, Toulouse, France: Effect of surfactants on multiphase flows
University of Valenciennes, France: Electrodiffusion diagnostics of the flow
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)

Visitors

N. Menuier, Institut National Polytechnique de Toulouse, France (Intership)
Ch. Faure-Llorens, Institut National Polytechnique de Toulouse, France (Intership)
J.-B. Henry, Institut National Polytechnique de Toulouse, France (Intership)
J. Conté, Institut National Polytechnique de Toulouse, France (Intership)
M. Azevedo, University of Minho, Braga, Portugal, (Intership)
S. Grillo, Universita degli Studi di Napoli Federico II., Italy (Erasmus)
R. Lau Wai Man, Nanyang Technological University, Singapore
V.V. Buwa, Indian Institute of Technology-Delhi, India
A .Byalko, Russian Acad.Sci., Landau Institute, Chernogolovka, Russia
H.A. Jakobsen, Norwegian University of Sci. and Technol.,Trondheim, Norway

Teaching

J. Drahoš, M. Růžička: ICT, Faculty of Chemical Engineering, postgraduate course "Multiphase Reactors"
J. Havlica: UJEP, Faculty of Science, course "Mathematics", "Petrochemistry"
J. Tihon, J. Vejražka: ICT, Faculty of Chemical Engineering, postgraduate course "Bubbles, drops, and particles"

Publications

Original papers

[1] Ait Mouheb N., Montillet A., Solliec C., Havlica J., Legentilhomme P., Comiti J., Tihon J.: Flow Characterization in T-Shaped and Cross-Shaped Micromixers. *Microfluid. Nanofluid.* 10(6), 1185-1197 (2011).

[2] Pěnkavová V., Tihon J., Wein O.: Stability and Rheology of Dilute TiO_2 – Water Nanofluids. *Nanoscale Res. Lett.* 6(1), 273 (2011).

[3] Poloncarzová M., Vejražka J., Veselý V., Izák P.: Effective Purification of Biogas by Condensing-Liquid Membrane. *Angew. Chem.-Int. Edit.* 50(3), 669-671 (2011).

[4] Sobolík V., Jirout T., Havlica J., Kristiawan M.: Wall Shear Rates in Taylor Vortex Flow. *J. Appl. Fluid Mech.* 4(3), 25-31 (2011).

[5] Stanovský P., Růžička M., Martins A., Teixeira J.A.: Meniscus Dynamics in Bubble Formation: A Parametric Study. *Chem. Eng. Sci.* 66(14), 3258-3267 (2011).

[6] Šimčík M., Mota A., Růžička M., Vicente A., Teixeira J.: CFD Simulation and Experimental Measurement of Gas Holdup and Liquid Interstitial Velocity in Internal Loop Airlift Reactor. *Chem. Eng. Sci.* 66(14), 3268-3279 (2011).

[7] Wein O., Tovčigrečko V.: Voltage-Step Transient on Circular Electrodes. *J. Appl. Electrochem.* 41(9), 1065-1075 (2011).

International conferences

[8] Basařová P., Hubička M., Vejražka J.: Influence of Bubble Surface Mobility on Motion of a Spherical Bubble in Neighbourhood of a Falling Particle. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 212-221, Tatranské Matliare, Slovakia, 23-27 May 2011.

[9] Baszczyński M., Novák P., Brányik T., Růžička M., Zedníková M.: Effect of Different Hop Extracts on Beer Foam Quality. 8th European Congress of Chemical Engineering, Programme, P44.27, Berlin, Germany, 25-29 September 2011.

[10] Fialová M., Orvalho S.P., Zedníková M., Drahoš J., Růžička M.: Effect of Electrolytes on Mass Transfer and Hydrodynamics in Bubble Column Operated in Homogeneous and Heterogeneous Conditions. 10th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Book of Abstracts, p. 55, Braga, Portugal, 26-29 June 2011.

[11] Kulaviak L., Hladil J., Růžička M., Drahoš J., Saint-Lary L.: Struktura vápencového sedimentu. (Czech) Structure of Sedimentary Calcite. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 80 (D3.1), Srní, Šumava, Czech Republic, 24-27 October 2011.

[12] Kulaviak L., Hladil J., Růžička M., Drahoš J.: Patterns Formation in Sedimentary Deposit. 10th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Book of Abstracts, p. 35, Braga, Portugal, 26-29 June 2011.

[13] Novák Pavel, Baszczyński M.: Influence of Wettability of Container Wall on Beer Foam Structure and Stability. 8th European Congress of Chemical Engineering, Programme, P44.05, Berlin, Germany, 25-29 September 2011.

[14] Novák Pavel, Baszczyński M., Brányik T., Růžička M., Zedníková M., Drahoš J.: Effect of Container Wall Properties on Beer Foam. 33rd European Brewery Convention Congress, Poster Abstracts, P34, Glasgow, Great Britain, 22-26 May 2011.

[15] Orvalho S.P., Růžička M.: Effect of the Bubble Characteristics on the Validity of Transition Concentration for Coalescence Behaviour of Electrolyte Solutions. 10th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Book of Abstracts, p. 28, Braga, Portugal, 26-29 June 2011.

[16] Pěnkavová V., Večeř M., Wein O.: AWS viskozimetrie mikrodisperzí - detekce zdánlivého skluzu na stěně. (Czech) AWS Viscosimetry of Microdispersions - Detection of Apparent Wall Slip. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, 6 pp. full text on CD-ROM, p. 47 (B2.3), Srní, Šumava, Czech Republic, 24-27 October 2011.

[17] Poloncarzová M., Vejražka J., Veselý V., Izák P.: Effective Purification of Biogas by a Condensing-Liquid Membrane. 38th International Conference of Slovak Society of Chemical Engineering , Proceedings, p. 102, Tatranské Matliare, Slovakia, 23-27 May 2011.

[18] Stanovský P., Růžička M.: Oscilace mezifázového menisku při tvorbě bublin. (Czech) Oscillation of Interfacial Meniscus during the Formation of Bubbles. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 188 (V61), Srní, Šumava, Czech Republic, 24-27 October 2011.

[19] Stanovský P., Růžička M.: Motion and the Oscillation of Interphase Meniscus Inside an Orifice during bubble Formation. 8th Liquid Matter Conference, Conference Book, p. 113 (P7.113), Wien, Austria, 06-10 September 2011.

[20] Stanovský P., Růžička M., Drahoš J.: The Influence of Operational Conditions on the Meniscus Dynamics in Bubble Formation. 10th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Book of Abstracts, p. 18, Braga, Portugal, 26-29 June 2011.

[21] Šimčík M., Mota A., Růžička M., Vicente A., Teixeira J., Drahoš J.: CFD Simulation and Experimental Measurement of Gas Holdup and Liquid Interstitial Velocity in Internal Loop Airlift Reactor. 10th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Book of Abstracts, p. 70, Braga, Portugal, 26-29 June 2011.

[22] Šimčík M., Růžička M.: CFD simulace proudění v laboratorním airlift reaktoru. (Czech) CFD Simulation of Laboratory Scale Airlift Reactor Hydrodynamics. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 191 (V64), Srní, Šumava, Czech Republic, 24-27 October 2011.

[23] Tihon J., Pěnkavová V., Havlica J., Šimčík M.: The Transitional Regime of Backward-Facing Step Flows. Experimental Fluid Mechanics 2011, Proceedings, p. 1022-1039, Jičín, Czech Republic, 22-25 November 2011.

[24] Večeř M., Leštinský P., Wichterle K., Růžička M.: Bubble Rising in Countercurrent Flow. 12th International Conference on Multiphase Flow in Industrial Plants, Book of Abstracts, p. 11, Ischia, Napoli, Italy, 21-23 September 2011.

[25] Večeř M., Pěnkavová V., Wein O.: Rheometric Study of Apparent Wall Slip in Microdispersions. The Nordic Rheology Conference, Annual Transactions the Nordic Rheology Society, p. 307-312, Helsinki, Finland, 8-10 June 2011.

[26] Večeř M., Pěnkavová V., Wein O.: The Role of Apparent Wall Slip Effect in Experimental Rheology. 8th European Congress of Chemical Engineering, Programme, P14.07, Berlin, Germany, 25-29 September 2011.

[27] Večeř M., Wein O.: Rotational Vicometry under Apparent Wall Slip. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 471-478, Tatranské Matliare, Slovakia, 23-27 May 2011.

[28] Vejražka J., Vobecká L., Kantorová J., Zedníková M., Orvalho S., Tihon J.: Shape Oscillations of Attached Bubbles in Pure Liquids and in Surfactant Solutions. 64th Annual Meeting of the APS Division of Fluid Dynamics, Bulletin of the American Physical Society, 56 (18), p. 147-148, Baltimore, USA, 20-22 November 2011.

[29] Vejražka J., Vobecká L.: Oscilace bublin a kapek přichycených na jehle. (Czech) Oscillations of a Bubble Attached to a Capillary Tip. 58. Konference chemického a procesního inženýrství, Sborník, 8 pp. full text on CD-ROM, p. 29 (B1.6), Srní, Šumava, Czech Republic, 24-27 October 2011.

[30] Vobecká L., Vejražka J., Tihon J.: Experimentální studium oscilací bublin v roztocích různých surfaktantů. (Czech) Experimental Study of Bubble Oscillations in Solutions of Different Surfactants. 58.

Konference chemického a procesního inženýrství CHISA 2011, Sborník, 9 pp. full text on CD-ROM, p. 187 (V60), Srní, Šumava, Czech Republic, 24-27 October 2011.

[31] Vobecká L., Vejražka J., Zedníková M., Orvalho S.P., Tihon J.: Oscillations of a Bubble Attached to a Capillary Tip in Solution of non-Ionic Surfactant. (Eng) 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 586–594, Tatranské Matliare, Slovakia, 23-27 May 2011.

[32] Vobecká L., Zedníková M., Vejražka J., Růžička M.: Experimental and Theoretical Study of Bubble Interactions with the Solid Surface. 10th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Book of Abstracts, p. 30, Braga, Portugal, 26-29 June 2011.

[33] Wein O.: AWS Viscometry – Principles and Applications. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, 18 pp. full text on CD-ROM, p. 46 (B2.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[34] Wein O.: A New Look on the Nernst Model in Electrochemistry. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 124 (C5.3), Srní, Šumava, Czech Republic, 24-27 October 2011.

[35] Wein O., Večeř M., Tihon J., Pěnkavová V.: AWS Viscometry - Principles and Applications. Novel Trends in Rheology IV, Novel Trends in Rheology IV, pp. 127-146, Zlín, Czech Republic, 27-28 July 2011.

Department of Organic Synthesis and Analytical Chemistry

HEAD
JAN SÝKORA

DEPUTY
JAN ČERMÁK

RESEARCH STAFF
MILENA BÁRTLOVÁ, VRATISLAV BLECHTA, PETRA CUŘÍNOVÁ, LUCIE ČERVENKOVÁ ŠŤASTNÁ, RÁMÍ DIMITROV, JINDŘICH KARBAN, ALENA KRUPKOVÁ, GABRIELA KUNCOVÁ, MILAN KURFÜRST, EVA MACHÁČKOVÁ, LUCIE MAIXNEROVÁ, JAN STORCH, STANISLAV ŠABATA
Part time: JIŘÍ HETFLEJŠ, JAN HORÁČEK, JAN SCHRAML, LUDMILA SOUKUPOVÁ

PHD STUDENTS
RENATA RYCHTÁRIKOVÁ, ANDREY SOLOVYEV, TOMÁŠ STRAŠÁK, HANA VRBOVÁ

TECHNICAL STAFF
JARMILA KUBEŠOVÁ

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
- Dehydrocoupling reactions catalyzed by titanium complexes
- Structure of silyl moieties through $J(^{29}Si\text{-}^{13}C)$ couplings as determined by triple $\{^{1}H, ^{13}C\}^{29}Si$ NMR experiment
- Synthesis of helicene derivatives
- Fluorinated carbosilane metallodendrimers

Applied research

- Enzymatically catalyzed synthesis of alkyd resins
- Development of new analytical methods
- Analytical services to the research departments of ICPF

Research projects

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

(G. Kuncová, kuncova@icpf.cas.cz; supported by MEYS, KONTAKT, project No. ME 892)

The research has been focused on inorganic and organic-inorganic matrices, which are employed in design of whole cell optical fiber sensors, and on physiology of microorganisms immobilized inside these matrices. [Refs. 15, 23, 35, 36]

Whole cell optical sensors (WOCOS)

(G. Kuncová, kuncova@icpf.cas.cz; supported by MEYS, KONTAKT, project No. ME 893)

We demonstrated the model laboratory protocol of application of free cells of bioluminescent bioreporter *P. putida* TVA8 as a sensor of organic pollutants, which are dissolved in water. The heights of bioluminiscence maxima were proportional to toluene concentration in the range 0–26 mg L^{-1}. Twenty-three organic pollutants (10^3 × diluted saturated solutions) and the samples from wastewater treatment plant were tested as bioluminescent inducers. *P. putida* TVA8 do not respond in a linear manner, hence there is no direct correlation with the chemical concentration. However, after range finding, as is the case for chromatographic analysis, the luminescence values can be related to a dose–response curve. [Refs. 8, 9, 12]

BIO-OPT-XUV (BOX) Research Team Advancement at the Faculty of Biomedical Engineering, Czech Technical University in Prague

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

The aim of this project is to strengthen education and research with a focus on the interactions of the optical (OPT) and the extreme ultraviolet (XUV) radiation with biological objects (BIO), and to further build up a research team at the FBME/CTU.

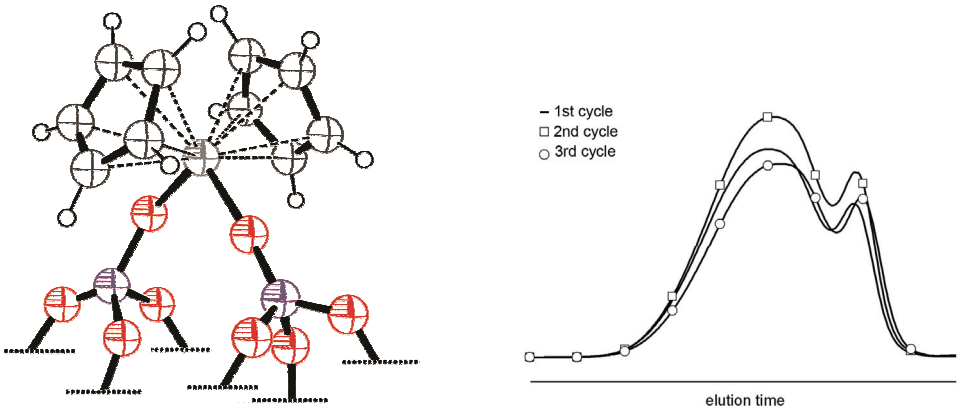
As a result, new innovative young academic workers (PhD and Master candidates in the fields of "Instruments and methods for biomedicine") will be integrated into the existing team; the post-graduate education in this field will be updated, the existing XUV FBME laboratory's international collaborative research will be advanced, and its infrastructure will be fortified by the introduction of new topics and methods.

Dehydrocoupling reactions catalyzed by titanium complexes

(J. Sýkora, sykora@icpf.cas.cz; joint project with JH IPC, and ICT, supported by GACR, grant No. 203/09/1574)

A series of zirconocene-siliceous catalysts were prepared and their catalytic performance and reusability was tested. [Refs. 4]

Products of dehydrocoupling polymerization reactions were monitored by advanced NMR techniques. The ^{1}J and ^{2}J ^{29}Si INADEQUATE experiments were used to reveal the connectivities within oligosilane chains. The presence of the branched oligophenylsilanes was confirmed. Furthermore, the formation of silyl-substituted cyclic oligomers and the presence of branched oligophenylsilanes in the catalytic systems studied by other authors were discussed. [Refs. 24-27]



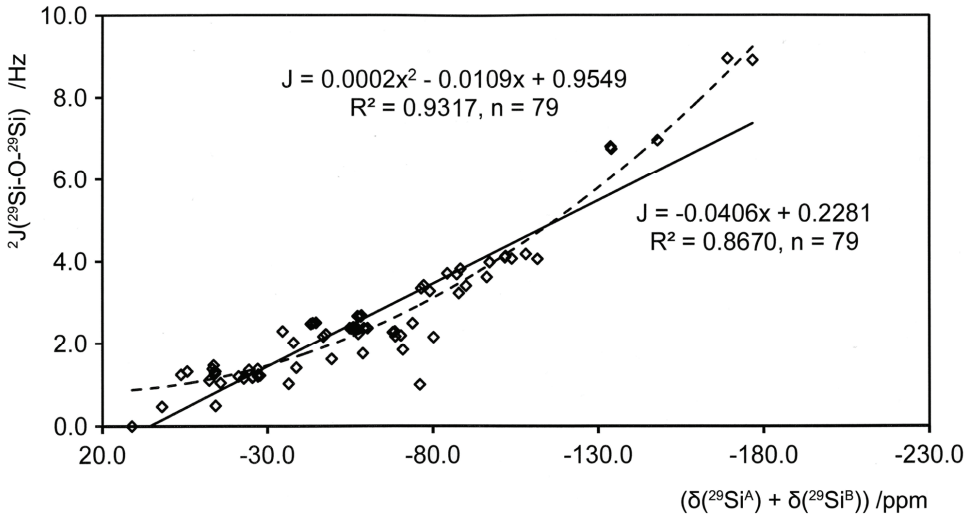
Analysis of Phenylsilane Polymers by Advanced ^{29}Si NMR

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, schraml@icpf.cas.cz; supported by GA ASCR, grant No. IAA400720706)

Within the project new methods for measurement of spin-spin couplings of ^{29}Si and ^{13}C nuclei in solutions were developed. The two most significant results include "Geminal ^{2}J(^{29}Si-O-^{29}Si) couplings in oligosiloxanes and their relation to direct ^{1}J(^{29}Si-^{13}C) couplings" [Ref. 10] and "2D correlation spectra edited by the sign of relative coupling constant" [Ref. 1]. In the first of these two papers the values and signs of geminal spin-spin coupling constants ^{29}Si-O-^{29}Si of industrially important siloxanes were published for the first time. Using 75 constants determined in 55 compounds under identical conditions it was shown that these constants are positive and correlate with one-bond ^{1}J(^{29}Si-^{13}C) couplings, with ^{29}Si chemical shifts and number of oxygenous substituents on the two silicon atoms involved.

In the second paper two new (CSEc and CSEh) pulse sequences were proposed. They allow editing of heteronuclear correlation spectra according to the signs of the selected heteronuclear coupling constants. The information about magnitude of the couplings is preserved. The methods achieve the sensitivity of E.COSY-type experiment. [Ref. 16, 17, 30-32].

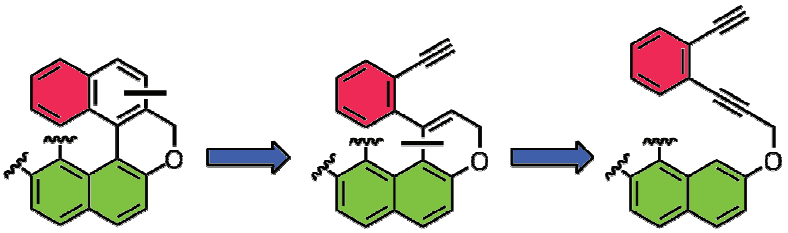


Dependence of ^{2}J(^{29}Si-O-^{29}Si) coupling between silicon nuclei Si^{A} and Si^{B} on the sum of their chemical shifts

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

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

Cycloisomerization of enynes catalyzed by complexes of transition metals represents simple, safe, and convenient to perform even on a larger scale, and therefore meet many of the stringent criteria imposed upon contemporary organic synthesis. In pursuit of our previous investigations in this field, we have described an alternative approach to helicene-like molecules based on a $PtCl_x$ catalyzed tandem cycloisomerization reaction. Its retrosynthetic approach is depicted below. [Refs. 37, 38]

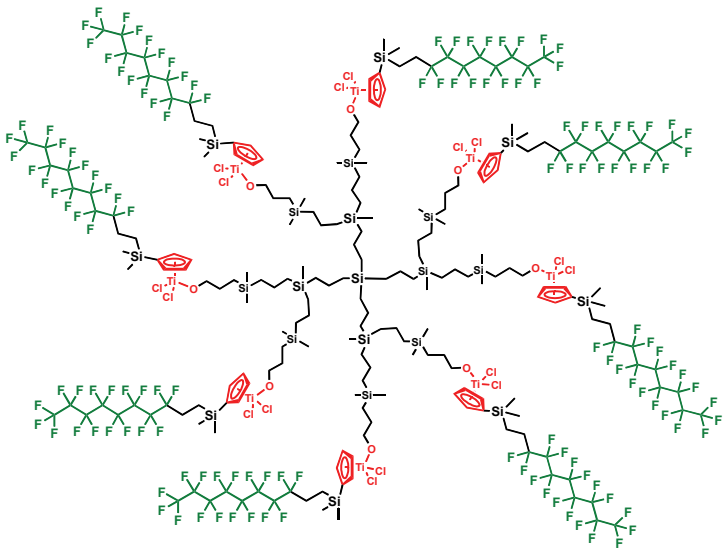


Retrosynthesis of tandem cycloisomerization leading to helicene-like molecules

The structure and synthetic applications of transition metal complexes

(J Čermák, cermak@icpf.cas.cz; supported by MYES, project No. LC06070)

Dehydration of (perfluoroalkyl)tetramethylcyclopentenols which are the precursors to (perfluoroalkyl)tetramethylcyclopentadienes was studied in detail including kinetic analysis. The principal reaction products are *endo-endo* and *endo,exo* isomers of the cyclopentadienes and some of them are formed by consecutive isomerization from other isomers. Dendritic polyols of the second and third generation were prepared by hydroboration/oxidation, of allyl-terminated carbosilane dendrimers and used as supports for immobilization of cyclopenta-dienyltrichlorotitanium(IV) complexes through alcoholysis. Reaction of dendrimers with $CpTiCl_3$ gave metallodendrimers with eight or sixteen $OTiCpCl_2$ units, whereas the reaction with $CpSiFTiCl_3$ ($CpSiF = C_5H_4SiMe_2CH_2CH_2C_8F_{17}$) provided peripherally fluorinated metallodendrimers. [Refs. 2, 18, 19, 21, 34]



Fluorinated metallodendrimer

Enzymatically catalyzed synthesis of alkyd resins (ENZALKYD)

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

The project is aimed at application of regioselective lipase type enzyme catalysts in the first step of alkyd resin synthesis, so called alcoholysis, which is based on reesterification of vegetable oils with low molecular weight polyols. The used enzymes will be studied in immobilized form on solid organosilicate polymeric carriers. The developed technology of innovated production of alkyd resins will be more environmentally friendly, will lower cost and energy demands, will improve security of work, and help to form new or better quality products, and thus will increase the competitiveness of Czech products on the European market.

Enzymatic glycerolysis of soybean oil catalyzed with the commercial lipase catalyst Novozym 435 has been carried out at 45-52 °C in a stirred tank and fixed-bed reactor, using *tert*-butyl alcohol as a solvent. The effects of reaction conditions on the glycerolysis were evaluated and optimum parameters found for the monoacylglycerol (MAG) production (yield > 85 %). Unlike the batch glycerolysis, in the packed bed reactor, the catalyst retained its activity in long-term operation, regardless of the reaction conditions used. The continuous transesterification of the oil with trimethylolpropane (TMP) afforded a mixture of monoacyl- and diacylglycerols in 90 % yield. The high yield of monoacyl-TMP (71 %) along with 24 % of 1-monoacyl- and 5 % of 2-monoacylglycerol gives evidence of the efficiency of the process. [Ref. 3]

International co-operations

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

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

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

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

Teaching

J. Čermák: UJEP, Faculty of Science, courses “Organic chemistry I and II”, “Chemistry of heterocyclic and organometallic compounds”, “Introduction to the spectral methods in organic chemistry”

G. Kuncová: ICT, Faculty of Chemical Engineering, postgraduate course “Optical sensors for measurement in chemical and biological reactors”

Publications

Original papers

[1] Blechta V., Schraml J.: 2D Correlation Spectra Edited by the Sign of Relative Coupling Constant. *Magn. Reson. Chem.* 49(3), 111-116 (2011).

[2] Čermák Jan, Nguyen Thi T.H., Včelák J., Krupková A.: Dehydration of (Perfluoroalkyl)tetramethyl-cyclopentenols. *Molecules* 16(5), 4031-4044 (2011).

[3] Hetflejš J., Šabata S., Sýkora J., Kuncová G., Vlček T.: Kontinuálně enzymová glycerolýza sojového oleje. (Czech) Continuous Enzymatic Glycerolysis of Soybean Oil. *Chem. Listy* 105(9), 684-690 (2011).

[4] Horáček M., Merna J., Gyepes R., Sýkora J., Kubišta J., Pinkas J.: Titanocene and ansa-Titanocene Complexes Bearing 2,6-bis(Isopropyl)Phenoxide Ligand(s). Syntheses, Characterization and Use in Catalytic Dehydrocoupling Polymerization of Phenylsilane. *Collect. Czech. Chem. Commun.* 76(1), 75-94 (2011).

[5] Chlebek J., Macáková K., Cahlíková L., Kurfürst M., Kuneš J., Opletal J.: Acetylcholin-esterase and Butyrylcholinesterase Inhibitory Compounds from *Corydalis cava (Fumariaceae)*. *Nat. Prod. Commun*. 6(5), 607-610 (2011).

[6] Kubec R., Krejčová P., Šimek P., Václavík L., Hajšlová J., Schraml J.: Precursors and Formation of Pyrithione and Other Pyridyl-Containing Sulfur Compounds in Drumstick Onion, Allium stipitatum. *J. Agric. Food. Chem.* 59(10), 5763-5770 (2011).

[7] Kučerová P., Kubec R., Šimek P., Václavík L., Schraml J.: Allium Discoloration: The Precursor and Formation of the Red Pigment in Giant Onion (*Allium giganteum Regel*) and Some Other *Subgenus Melanocrommyum Species*. *J. Agric. Food Chem.* 59(5), 1821-1828 (2011).

[8] Kuncová G.: Optický biosenzor pro reaktory. (Czech) Optical Biosensor for Reactors. *Vesmír* 90(6), 345 (2011).

[9] Kuncová G., Pazlarová J., Hlavatá A., Ripp S., Sayler G.S.: Bioluminescent Bioreporter *Pseudomonas putida TVA8* as a Detector of Water Pollution. Operational Conditions and Selectivity of Free Cells Sensor. *Ecol. Indic.* 11(3), 882-887 (2011).

[10] Kurfürst M., Blechta V., Schraml J.: Geminal $^{2}J(^{29}\mathrm{Si\text{-}O\text{-}}^{29}\mathrm{Si})$ Couplings in Oligosiloxanes and Their Relation to Direct $^{1}J(^{29}\mathrm{Si\text{-}}^{13}\mathrm{C})$ Couplings. *Magn. Res. Chem.* 49(8), 492-501 (2011).

[11] Magalhaes P.J., Carvalho A.B., Goncalves L.M., Pacheco J.G., Guido L.F., Brányik T., Rodrigues P.G., Kuncová G., Dostálek P., Barros A.A.: The Impact of Xamthohumol on a Brewing Yeast's Viability, Vitality and Metabolite Formation. *J. Inst. Brew.* 117(3), 368-376 (2011).

[12] Rychtáriková R., Kuncová G.: Metoda vyhodnocování antimikrobiální aktivity počítačovým prahováním barev. (Czech) Assessment of Antimicrobial Activity via Computational Tresholding of Colours. *Chem. Listy* 105(6), 493-498 (2011).

[13] Schraml J., Kubec R., Kučerová P.: Determination of Substitution Sites in Monosubstituted Five-Membered Aromatic Heterocycles. *Magn. Reson. Chem.* 49(3), 147-150 (2011).

[14] Topka P., Karban J., Soukup K., Jirátová K., Šolcová O.: Preparation of Al-SBA-15 Pellets with Low Amount of Additives: Effect of Binder Content on Texture and Mechanical Properties. Application to Friedel-Crafts Alkylation. *Chem. Eng. J.* 168(1), 433-440 (2011).

Review papers

[15] Kuncová G., Trögl J.: Mikroorganismy imobilizované do anorganických nosičů. (Czech) Living Microorganisms Immobilized in Inorganic Matrices. *Chem. Listy* 105(11), 830-838 (2011).

International conferences

[16] Blechta V., Schraml J.: Detection of Signed Homonuclear Couplings between Low Abundant Nuclei. 26th NMR Vatltice, Book of Abstracts, C-16, Valtice, Czech Republic, 1-4 May 2011.

[17] Blechta V., Schraml J.: Detection of NMR Spectra Edited by Signs of Coupling Constants. Magnetic Moments in Central Europe, Program and Book of Abstracts, p. 16, Tatranská Lomnica, Slovakia, 16-20 March 2011.

[18] Čermák Jan, Strašák T.: Carbosilane Dendrimers Decorated with Titanocene Dichloride. 7th International Dendrimer Symposium, Program and Abstracts, p. 63 (B1.5), Gaithersburg, Maryland, USA, 26 June - 1 July 2011.

[19] Čermák Jan, Strašák T.: Titanocene Dichloride Immobilization on Carbosilane Dendrimers. 19th EuCheMS International Conference on Organometallic Chemistry, Book of Abstracts, P008, Toulouse, France, 3-7 July 2011.

[20] Kaluža L., Sýkora J., Karban J., Žáček P., Vít Z., Zdražil M.: Hydrodesulfurization of Model Feed Containing Olefins over Al_2O_3, TiO_2, and ZrO_2 Supported Transition Metal Sulfides. 8th European Congress of Chemical Engineering, Programme, P19.01, Berlin, Germany, 25-29 September 2011.

[21] Krupková A., Čermák Jan: Carbosilane Titanium Metallodendrimers with Polyfluoroalkylated Cyclopentadienyl Ligands. International Symposium on Fluorous Technologies 2011 (ISoFT'11), Programme and Abstracts, P-8, Hong Kong, Hongkong, 30 November - 3 December 2011.

[22] Křišťál J., Drhová M., Jiřičný V., Kuncová G.: Microreactor Flow System for Enzymatic Reactions. CAMURE-8 & ISMR-7, Book of Abstracts, p. 149, Naantali, Finland, 22-25 May 2011.

[23] Kuncová G., Šabata S., Kučerová L., Fuzik T., Duchek P.: Lipases in Hierarchically Structured Montmorillonite. XIXth International Conference on Bioencapsulation, Posters, pp. 116-117, Amboise, France, 5-8 October 2011.

[24] Pinkas J., Blechta V., Karban J., Sýkora J.: Analysis of Phenylsilane Polymers by Advanced ^{29}Si NMR. Magnetic Moments in Central Europe 2011, Program and Book of Abstracts, Tatranská Lomnica, Slovakia, 16-20 March 2011.

[25] Pinkas J., Blechta V., Karban J., Sýkora J.: ^{29}Si NMR Phenylsilane Polymer Analysis. 26th NMR Vatltice, Book of Abstracts, C-20, Valtice, Czech Republic, 1-4 May 2011.

[26] Pinkas J., Merna J., Sýkora J.: LC-NMR Analysis of Phenylsilane Polymers. 43rd Symposium on Catalysis, Program and Book of Abstracts, Praha, Czech Republic, 7-8 November 2011.

[27] Pinkas J., Merna J., Sýkora J.: From Nanocatalysts to Reusable Heterogeneous Catalysts in Phenylsilane Dehydropolymerization. Zing Nanomaterials Conference 2011, Abstracts - Posters, p. 66 (P11), Xcaret, Mexico, 28 November - 02 December 2011.

[28] Sajfrtová M., Pavela R., Karban J.: Vliv podmínek superkritické extrakce na insekticidní účinky výtažků z routy vonné. (Czech) Effect of Conditions of Supercritical Fluid Extraction on Insecticidal Activity of Isolates from Rue. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 166 (V39), Srní, Šumava, Czech Republic, 24-27 October 2011.

[29] Sajfrtová M., Rochová K., Karban J., Sovová H., Pavela R.: Supercritical Fluid Extraction of Botanical Insecticides from Rue. 11th International Conference on Carbon Dioxide Utilization, Program and Abstracts, p. 207, Dijon, France, 27-30 June 2011.

[30] Schraml J., Kurfürst M., Blechta V.: Geminal Spin-Spin $^2J(^{29}\text{Si-O-}^{29}\text{Si})$ Couplings in Silicones and Silicates. 16th International Symposium on Silicon Chemistry, Program/Abstract Book, 171, Hamilton, Ontario, Canada, 14-18 August 2011.

[31] Schraml J., Kurfürst M., Blechta V.: Empirical and Not-so-Empirical Correlations Holding for $^2J(^{29}\text{Si-O-}^{29}\text{Si})$ Couplings in Industrially Important Siloxanes. 26th NMR Vatltice, Book of Abstracts, C-19, Valtice, Czech Republic, 1-4 May 2011.

[32] Schraml J., Kurfürst M., Blechta V.: The Relative Signs of Coupling Constants from Inadequate Experiment of Equivalent Nuclei - an Educational Example. Magnetic Moments in Central Europe, Program and Book of Abstracts, p. 20, Tatranská Lomnica, Slovakia, 16-20 March 2011.

[33] Schwarz J., Karban J., Chalupníčková E., Pokorný R., Novák J., Smolík J.: The Influence of Biomass Burning on PM2.5 at Urban and Rural Background Sites in the Czech Republic. European Aerosol Conference EAC 2011, Book of Abstracts, p. 899 (4P306), Manchester, Great Britain, 4-9 September 2011.

[34] Strašák T., Čermák J.: Carbosilane Dendrimers Containing Titanium Complexes on Their Periphery. 13th International Seminar of PhD Students on Organometallic and Coordination Chemistry, Book of Abstracts, OP6, Liblice, Czech Republic, 3-7 April 2011.

[35] Šabata S., Hetflejš J., Kuncová G., Macháčková E.: Continuous Transesterification Catalyzed with Immobilized Lipase. XIXth International Conference on Bioencapsulation, Posters, pp. 118-119, Amboise, France, 5-8 October 2011.

[36] Šabata S., Kuncová G., Hetflejš J., Lhoták P., Slavíček J.: Porphyrin Composite Materials for Fullerene Separation. Zing Nanomaterials Conference 2011, Abstracts - Posters, p. 64 (P9), Xcaret, Mexico, 28 November - 2 December 2011.

[37] Barták Z., Bernard M., Sýkora J., Storch J.: Exploration of Tandem Cycloizomerization Leading to Tetrahydro[8]helicene. 23rd International Symposium on Polycyclic Aromatic Compounds ISPAC 23, Abstracts, p. 35, Münster, Germany, 04-08 September 2011.

[38] Bernard M., Sýkora J., Storch J.: Design and Synthesis of Helicene like Molecules. 43rd Symposium on Catalysis, Program Book of Abstracts, P04A, Praha, Czech Republic, 07-08 November 2011.

Environmental Process Engineering Laboratory

HEAD
MIROSLAV PUNČOCHÁŘ

DEPUTY
VLADIMÍR CÍRKVA

RESEARCH STAFF
VÁCLAV GRUBER, MIROSLAV HARTMAN, PETRA KAMENÍKOVÁ, MICHAEL POHOŘELÝ, KAREL SVOBODA, MICHAL ŠYC, OTAKAR TRNKA, LEONA VLKOVÁ
Part time: EVA FIŠEROVÁ, MILAN HÁJEK, VÁCLAV VESELÝ

PHD STUDENTS
JAN ČERMÁK, MICHAL JEREMIÁŠ, STANISLAV RELICH, JIŘÍ SOBEK

TECHNICAL STAFF
JAROSLAV BRUSTMANN, OLEKSIY KHRAMKOV, MARTIN KRČEK, VLADIMÍR POMYKAČ, MARKÉTA TOŠNAROVÁ

Fields of research

- Electrodeless discharge lamps for photochemistry and photocatalysis in microwave field
- Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis
- Effect of microwaves on selective leaching of Pb, Zn and Al from the electronics waste
- Fluidization and decontamination of organic-polluted solids in a fluid-bed reactor
- Fluidized bed incineration of dry sewage sludge from the waste water treatment plant
- Advanced processes for gasification, gas cleaning and hydrogen production
- Persistent organic pollutants and heavy metals from small sources

Applied research

- Fluidized bed combustion and gasification
- Moving bed gasification of wood and waste wood
- Development and verification of thermal desorption technology using microwaves
- Brownfields - source of renewable energy
- Waste and sewage sludge combustion and co-combustion
- Simultaneous microwave drying and disinfection of flooded books
- Hydrogen production via synthetic gas by biomass/oil partial oxidation
- Method for obtaining extracts containing europium and yttrium and method for recovery of spent phosphors from compact fluorescent lamps

Research projects

Photochemistry and photocatalysis in the microwave field - overview

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

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

The objective of this discipline is frequently, but not necessarily, connected to the electrodeless discharge lamp (EDL) as a novel light source which generates efficiently UV/Vis radiation when placed into a microwave field. This review article is focused on the general principles of microwave photochemistry and photocatalysis, i.e. generation of UV/Vis discharge in EDL (theory of the microwave discharges, construction of EDL, preparation of the thin titania films on EDL, spectral characteristics of EDL, and performance of EDL). Likewise, the various microwave photochemical and photocatalytic reactor types (batch with external or internal light source, flow-through with external light source, annular flow-through with internal EDL, and cylindrical flow-through surrounded with EDL) with different arrangement of the lamps are described. The concept of microwave photochemistry and photocatalysis as an important issue in synthetic chemistry and material science is presented in several tables. [Refs. 1, 12]

Experimental set-up for microwave photochemistry and photocatalysis

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

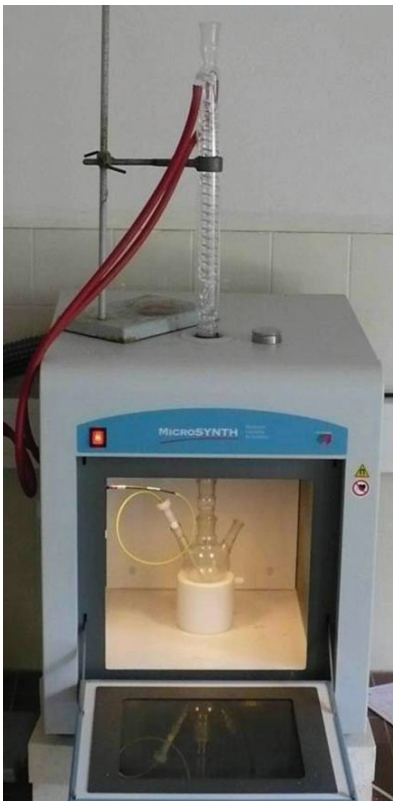
(M. Hájek, hajek@icpf.cas.cz; supported by GACR, grant No. 104/08/0416)

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. [Ref. 18]

Effect of microwave energy on selective leaching of Pb, Zn and Al from the electronics waste with high Cu contents

(M. Hájek, J. Sobek, hajek@icpf.cas.cz, sobek@icpf.cas.cz; joint project with Institute of Geotechnics of the SAS, Košice, Slovakia; supported by SAS, projects No. APVV-51-035505 and VEGA 02/0087/08)

The project deals with the use of conventional and microwave-assisted leaching of copper, aluminium, zinc and lead from electronics scrap using 2 M HCl. The method has been investigated to improve the yields of extracted metals and to reduce the processing time. The leaching was carried out at the boil of the acid. The experiments were performed in a modified microwave oven, applying a full factorial design involving the acid concentration, the liquid/solid ratio and irradiation time. The impact factors and their interactions affecting the metal yields were different. The maximum recovery of Al, Zn, Pb was up to 90 % at 30-min leaching. The dissolution of Cu was negligible. The yields of Pb and Al were dependent on temperature, time and the method of leaching. The yields were 91 % after 60 min of microwave heating at 60 °C, and 83 % in the case of conventional heating. At 80 °C virtually all Pb went into solution after 60-min microwave leaching, while the yield of the conventional leaching was only 60 %. [Ref. 11]



Microwave synthesis labstation MicroSYNTH (Milestone srl, Italy)

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

(M. Hartman, hartman@icpf.cas.cz; supported by GA ASCR, grant No. IAA400720701)

An ideally mixed flow model is developed for the high-temperature oxidation of toxic carbon monoxide into inert carbon dioxide occurring in an afterburner chamber. The extent of the oxidation reaction in oxygen – and water vapor – bearing flue gas is explored as a function of the relative throughput, the gas density, and the global rate of reaction. Steady-state experimental measurements of the CO, O_2, CO_2, and water vapor concentrations were conducted in a pilot-plant refractory afterburner fitted with a natural gas burner. The global burnout reaction is assumed to be first order in carbon monoxide and one-half order with respect to oxygen and water vapor. The numerical solutions of the model equations outline the possibilities and limitations for the performance of a well-mixed afterburner chamber (reactor) under realistic operating conditions. [Ref. 4]

Fluidized-bed incineration of dry sewage sludge from the waste water treatment plant in Brno-Modřice

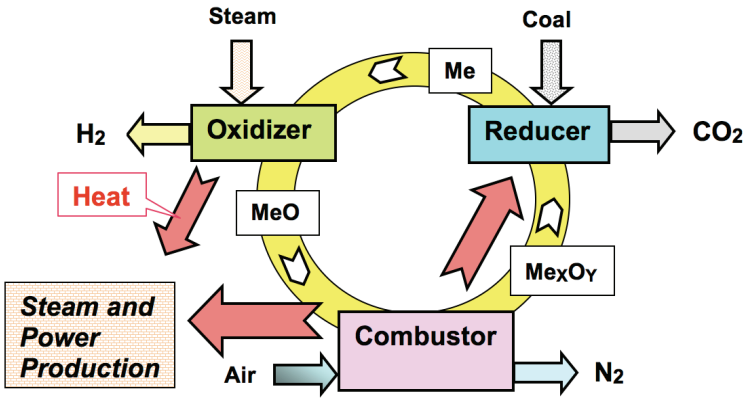
(M. Pohořelý, pohorely@icpf.cas.cz; contract with Brno University of Technology)

Contract devoted to experimental tests in the field of emission generation in sewage sludge incineration. Primarily, the experiment aimed at evaluating the influence of limestone addition to sludge incineration on the generation and removal of acidic components (hydrogen halides, sulfur dioxide). Additionally, further gaseous emissions as well as heavy metals were explored. The results were evaluated on the basis of current legislation.

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

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

The bilateral research project is aimed at development of advanced fluidized bed gasification process with efficient gas cleaning and research of advanced processes for chemical looping technologies for hydrogen production. Barrier filters with fixed/moving bed of granular materials and dry methods for removal of sulfur and chlorine compounds are studied and further developed. Also effects of staging of gasification media and effects of fluidized bed particulate materials on gasification, tar destruction and limitation of sulfur compounds emissions are among subjects of bilateral research.



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

Emission factors of POPs and heavy metals from small sources

(M. Šyc, syc@icpf.cas.cz; joint project with Energy Research Center VŠB-TU Ostrava, Institute of Public Health in Ostrava; supported by Ministry of the Environment of the CR, project No. SP/1a2/116/07)

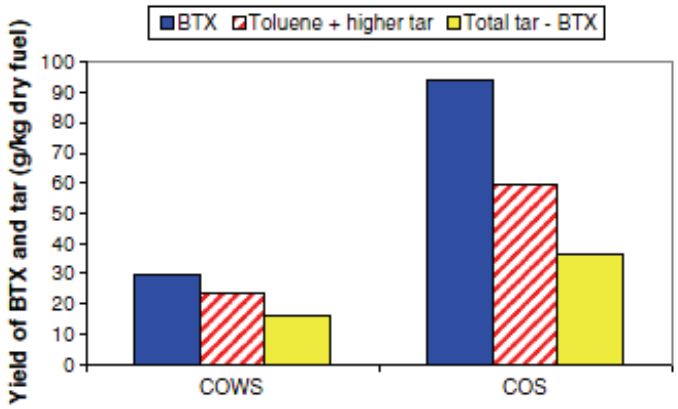
Domestic heating appliances are significant source of air pollution. The project reports on the first complex data set of emission factors (EFs) of selected pollutants from combustion of five fuel types (lignite, bituminous coal, spruce, beech, and maize) in six different domestic heating appliances of various combustion designs. The effect of fuel as well as the effect of boiler type was studied. Numerous EFs were measured, including the EFs of particulate matter (PM), carbon monoxide (CO), polyaromatic hydrocarbons (PAH), hexachlorobenzene (HxCBz), polychlorinated dibenzo-p-dioxins and furans (PCDD/F), etc. The obtained data set can be used for unambiguous recommendation of suitable heating appliances and fuels leading to minimization of environmental pollution. [Refs. 5, 7, 9, 16]

Czech village in winter season (photo by Jiří Horák)

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

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

The project aims at integrating gasification schemes for the co-gasification of coal, biomass and waste with processes for CO_2 separation and capture. Fluidized bed and entrained flow gasification processes are considered thanks to their flexibility and effectiveness for carrying out thermal conversion of different feedstock and for matching different requirements of producer gas end-users and for effective CO_2 separation. Fuel feeding in a form of solid particles, mixtures of solid particles and various slurries (suspensions of solid fuel particles) and different fluidized bed particulate materials (sand, dolomite, olivine) are compared in terms of their effects in fluidized bed gasification. Effects of both, primary measures (involved in overall conditions of a given gasification process) and secondary (downstream) measures on syngas properties (particularly composition, purity and heating value) and possible applications are studied. [Refs. 27, 28, 29, 30]

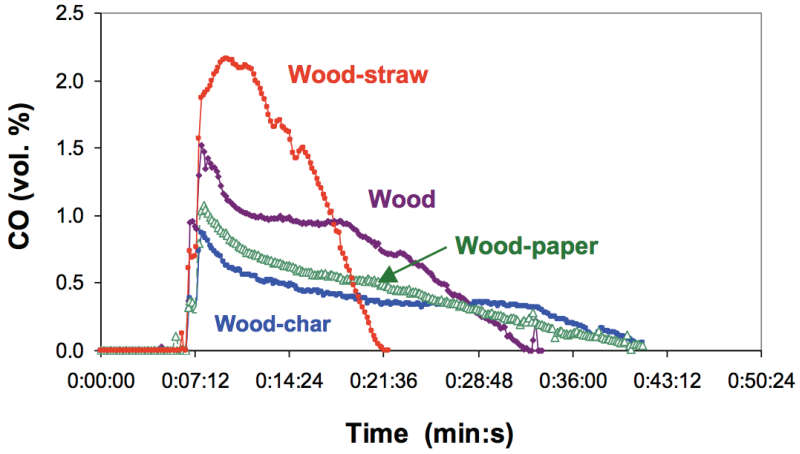


Comparison of BTX and tar yield from FB gasification of Polish coal based ternary slurry COWS (ER=0.19, CO_2/dry fuel mass ratio=2.39, H_2O/C molar ratio=0.7) at 850 °C and Polish coal based COS (ER=0.20, CO_2/dry fuel mass ratio=2.43)

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

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

Contract dealing with experimental support for development of a new type of moving bed gasifier (up-draft, co-current), production and testing of various biomass pellets for such gasification, experimental research of suitable conception for producer gas cleaning (mainly dry, adsorption based methods) and effects of air staging on tar concentration in produced gas. [Refs. 19, 30]



Comparison of CO_2 gasification rates of the four kinds of pellets in terms of measured CO concentrations in outlet gas

Development and verification of thermal desorption technology using microwave radiation

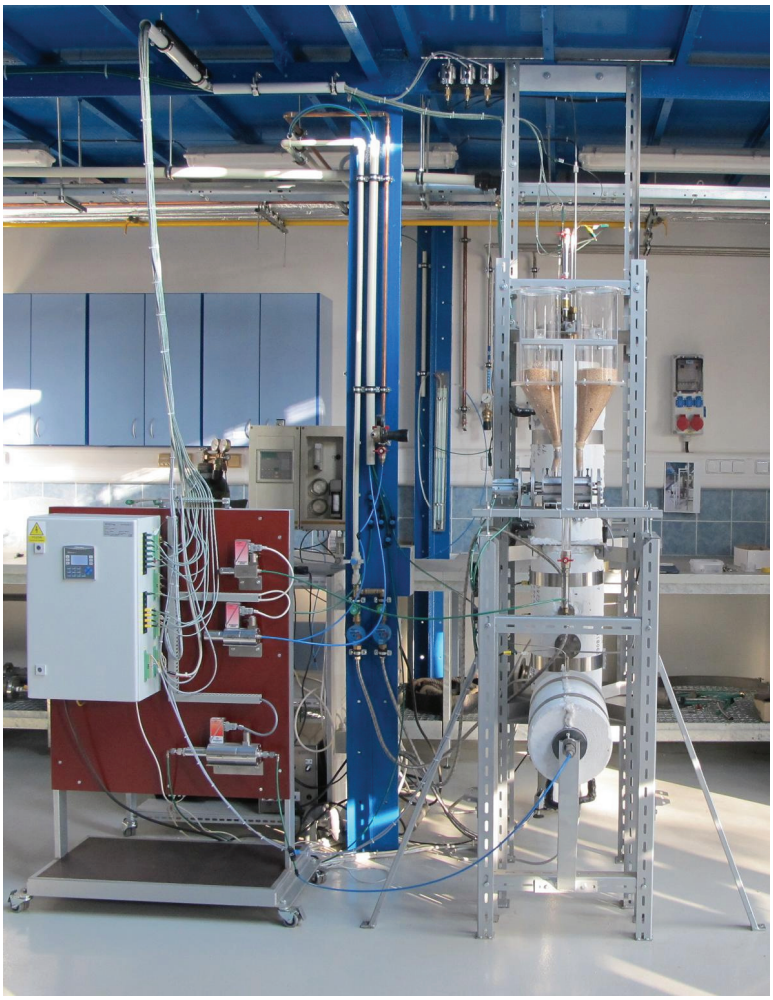
(M. Hájek, J. Sobek, hajek@icpf.cas.cz, sobek@icpf.cas.cz; joint project with ICT and Dekonta, a.s; supported by TACR, projects No. TA01020383)

The main goal of the project is development and verification of thermal treatment method utilizing microwave radiation for heating up contaminated material in a primary treatment unit. An originally designed pilot-scale treatment unit will be assembled. Operation efficiency of the unit will be verified by treatment of wide range of contaminated soil and solid waste samples. By development of this innovative technology, the applicant will strengthen his market position and improve his competitiveness in the field of remediation services and hazardous waste treatment activities. [Refs. 6, 23]

Brownfields - Source of renewable energy (BROZEN)

(M. Punčochář, M. Šyc, punc@icpf.cas.cz; syc@icpf.cas.cz; joint project with EVECO Brno Ltd., CULS Prague; supported by TACR, project No. 01020366)

The phytoextraction ability of some fast growing plant species leads to the idea of connecting biomass production with soil remediation of contaminated industrial zones and regions. This biomass will contain significant amount of heavy metals and its energetic utilization has to be considered carefully to minimize negative environmental impacts. Therefore, behavior of selected heavy metals was observed during fluidized bed gasification and combustion of contaminated biomass (willows, poplars, flax). This knowledge is essential for further utilization of all products of gasification and for the fulfillment of emission limits during combustion. [Refs. 10, 31, 32]

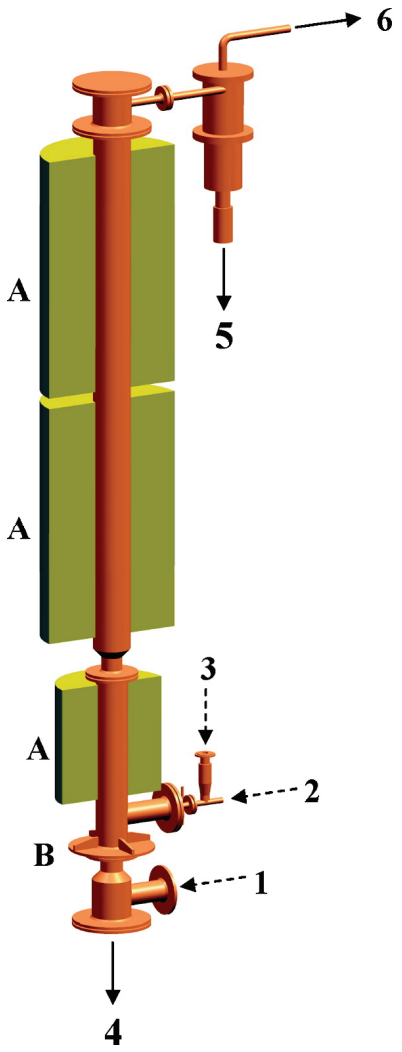


Fluidized bed reactor

Waste as raw material and energy source (WARMES)

(M. Punčochář, punc@icpf.cas.cz; joint project with Brno University of Technology, EVECO Brno Ltd.; 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. 10, 14, 15, 20, 25]



A - Heating

B - Grate

1 - Pre-heated gasification agent (steam+nitrogen)

2 - Nitrogen for pneumatic transport

3 - Blended fuel

4 - Bed ash

5 - Cyclone ash

6 - Producer gas

- solid phase of fly ash

- gaseous phase

Scheme of fluidized bed reactor

Simultaneous microwave drying and disinfection of flooded books

(M. Hájek, hajek@icpf.cas.cz; joint project with ICT and National Archives of the CR;
supported by ASCR, grant No. AV0Z40720504)

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. Almost all books and documents were dried without any damage to printing in metallic inks, colored reproductions, metallic objects and other components sensitive to microwaves. The treatment also destroyed moulds and their spores by use of UV electrodeless lamps, which rendered additional disinfection unnecessary. [Ref. 2]

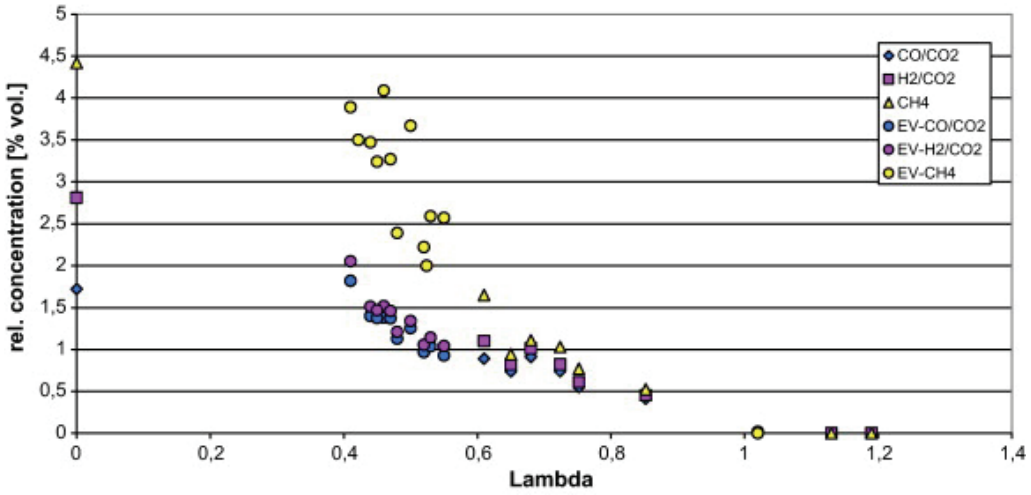
Continuous microwave drying equipment

Hydrogen production via synthetic gas by biomass/oil partial oxidation

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

Common research efforts of ICPF, Institute of Inorganic Chemistry Ústí n/L and ICT Prague were focused on comparison of pilot plant partial oxidation of meal rape and hydrocarbon oil mixture with process simulation using equilibrium reactor model by process simulator Aspen Plus which resulted in a good agreement. The application of representative compounds method for simulation of such complex mixture was found as a useful tool for optimal process conditions prediction. Based on this procedure the ratio feed to both oxygen and steam were proposed for prediction of good experimental parameters for good process yield of hydrogen. The advantage of co-gasification of bio-waste and hydrocarbon oil mixture using suspension of 10 wt% meal rape in the feed can be observed in higher hydrogen production in cca 2.5 % rel. and lower oxygen and steam process demand in cca 5 % rel. It was stated that key parameter lambda (or analogously oxygen to feed ratio) controlling the partial oxidation process in optimal regime should be in the interval 0.6–0.8, i.e. under reaction conditions.

Partial oxidation regime can be characterized by similar lambda parameter used e.g. in characterization of car engine regime. Lambda is the dimensionless ratio of actual quantities of oxygen into the reactor should amount to, in theory, the quantity of oxygen required for combustion of carbon in the fuel to CO_2 and hydrogen to water. Where fuel (biomass) contains oxygen, then this oxygen is considered a reactive and reduces the theoretical quantity of oxygen. If the fuel contains moisture, its oxygen does not count. The effect of small content of nitrogen and sulfur in the feed on oxygen demand was neglected. Regime of partial oxidation of the complex feed strongly influenced the product composition. Figure illustrates the effect of lambda parameter on different product components ratio in the product stream. This is experimental evidence of necessity to operate the process under the reduction conditions for lambda value interval 0.6–0.8. In case of more reduction regime the dominant production of methane was observed. [Refs. 3, 33-36]



Product composition versus gasification regime. Temperature 1200 °C; experiments with pure oil and (EV) with 8% meal rape content in hydrocarbon oil, resp.

Method for obtaining extracts containing europium and yttrium and method for recovery of spent phosphors from compact fluorescent lamps

(V. Gruber, gruber@icpf.cas.cz; supported by ICPF)

In the present invention, there is disclosed a method for obtaining extracts containing Eu and Y from raw material comprising acid inorganic aqueous spent liquors of luminophore concentrate when recycling color kinescopes and monitors wherein the method is based on countercurrent continuous extraction with subsequently w elutriation of extract with a diluted mineral acid from acid aqueous spent liquors containing inorganic acid and water, using an extraction agent consisting of bis-(2-etylhexyl)phosphoric acid and liquid aliphatic hydrocarbons wherein the method of the present invention is characterized in that obtained mixture is extracted in a extraction countercurrent column with two separating terminal sections and two inlets of aqueous phase and one inlet of organic phase. [Refs. 13, 17]

International co-operations

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

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

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

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

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

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

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

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

Visits Abroad

P. Kameníková: Hawaii Natural Energy Institute, University of Hawaii, USA (2 months)

Teaching

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

Publications

Original papers

[1] Církva V., Relich S.: Microwave Photochemistry and Photocatalysis. Part 1: Principles and Overview. *Curr. Org. Chem.* 15(2), 248-264 (2011).

[2] Hájek M., Ďurovič M., Paulusová H., Weberová L.: Simultaneous Microwave Drying and Disinfection of Flooded Books. *Restaurator* 31(1), 1-7 (2011).

[3] Hanika J., Lederer J., Tukač V., Veselý V., Kováč D.: Hydrogen Production via synthetic Gas by Biomass/Oil Partial Oxidation. *Chem. Eng. J.* 176-177(1), 286– 290 (2011).

[4] Hartman M., Trnka O., Veselý V., Svoboda K.: Termická oxidace oxidu uhelnatého ve spalných plynech. (Czech) Thermal Oxidation of Carbon Monoxide in Flue Gas. *Chem. Listy* 105(7), 546-552 (2011).

[5] Horák J., Hopan F., Šyc M., Machálek P., Krpec K., Ocelka T., Tomšej T.: Bilance emisí znečišťujících látek z malých zdrojů znečišťování se zaměřením na spalování tuhých paliv. (Czech) Estimation of Selected Pollutant Emissions from Solid-Fuel Combustion in Small Heating Appliances. *Chem. Listy* 105(11), 851-855 (2011).

[6] Kaštánek P., Kaštánek F., Hájek M., Sobek J., Šolcová O.: Dehalogenation of Polychlorinated Biphenyls (PCB) by Nucleofile Reactants at the Presence of Ionic Liquids and under Application of Microwaves. *Global NEST J.* 13(1), 59-64 (2011).

[7] Keppert M., Pavlík Z., Vejmelková E., Černý R., Šyc M.: Popeloviny ze spalovny komunálního odpadu jako alternativní palivo cementové malty. (Czech) Ash Materials from Municipal Solid Waste Incinerators as Alternative Filling Agent of Cement Mortar. *Stavební obzor* 20(3), 74-77 (2011).

[8] Poloncarzová M., Vejražka J., Veselý V., Izák P.: Effective Purification of Biogas by Condensing-Liquid Membrane. *Angew. Chem.-Int. Edit.* 50(3), 669-671 (2011).

[9] Šyc M., Horák J., Hopan F., Krpec K., Tomšej T., Ocelka T., Pekárek V.: Effect of Fuels and Domestic Heating Appliance Types on Emission Factors of Selected Organic Pollutants. *Environ. Sci. Technol.* 45(21), 9427-9434 (2011).

[10] Šyc M., Pohořelý M., Jeremiáš M., Vosecký M., Kameníková P., Skoblia S., Svoboda K., Punčochář M.: Behavior of Heavy Metals in Steam Fluidized Bed Gasification of Contaminated Biomass. *Energy and Fuels* 25(5), 2284–2291 (2011).

[11] Znamenáčková I., Lovás M., Hájek M., Sobek J.: Vplyv mikrovlnnej energie na selektívne lúhovanie Pb, Zn a Al z elektronického odpadu s vysokým obsahom Cu. (Slov) The Effect of Microwave Energy on Selective Leaching of Pb, Zn and Al from the Electronics Waste with High Cu Contents. *Chem. Listy* 105(5), 625-628 (2011).

Review papers

[12] Církva V., Relich S.: Microwave Photochemistry. Applications in Organic Synthesis. *Mini-Reviews in Organic Chemistry* 8(3), 282-293 (2011).

Patents

[13] Gruber V., Rousková M., Heyberger A., Staf M.: Způsob získávání extraktů s obsahem europia a yttria. (Czech) Method for Reclaiming of Organic Extracts Containing Europium and Yttrium Ions. Pat. No. *CZ302854/PV 2010-928*. Applied: 10.12.14, Patented: 11.12.14.

[14] Habart J., Tlustoš P., Balík J., Pavlíková D., Hanč A., Jelínek F., Pohořelý M., Punčochář M.: Soustava pro fermentaci pevné biomasy. (Czech) A System for Solid Biomass Fermentation. Pat. No. *CZ302733/PV 2010-620*. Applied: 10.08.17, Patented: 11.08.24.

[15] Habart J., Tlustoš P., Balík J., Pavlíková D., Hanč A., Jelínek F., Pohořelý M., Punčochář M.: Soustava pro fermentaci pevné biomasy. (Czech) A System for Solid Biomass Fermentation. Pat. No. *CZ21952/PUV 2010-23118*. Applied: 10.08.17, Patented: 11.03.21.

[16] Keppert M., Pavlík Z., Černý R., Šyc M.: Materiál pro imobilizaci těžkých kovů. (Czech) Material for Immobilization of Heavy Metals. Pat. No. *CZ22103/PUV 2010-23166*. Applied: 10.08.30, Patented: 11.04.21.

[17] Gruber V.: Způsob přepracování odpadních luminoforů z kompaktních fluorescenčních lamp. (Czech) Method for Recovery of Spent Phosphors from Compact Fluorescent Lamps (CFLs) . Pat. No. *PV 2011-298*. Applied: 11.05.18.

[18] Hájek M., Sobek J.: Způsob alkylace aromatických uhlovodíků. (Czech) Method of Alkylation of Aromatic Hydrocarbons . Pat. No. *PV 2011-486*. Applied: 11.08.09.

[19] Svoboda K., Smetana J., Štojdl J., Šulc J., Vacek J.: Způsob zplyňování upravené biomasy a zařízení k jeho provádění. (Czech) Method and Apparatus/Equipment for Gasification of Adapted Biomass. Pat. No. *PV 2011-404*. Applied: 11.07.01.

International conferences

[20] Cabáková G., Jeremiáš M., Pohořelý M.: Odstraňování halogenidů z generátorového plynu vzniklého zplyňováním biomasy. (Czech) Halide Removal from Syngas Derived from Biomass Gasification. 63. Zjazd chemikov, ChemZi 7(13), pp. 259-260, 2011, Tatranské Matliare, Vysoké Tatry, Slovakia, 5-9 September 2011.

[21] Čapek L., Smoláková L., Priecel P., Kutálek P., Hájek M., Bulánek R., Kubičková I., Matějová L.: Analysis of Basic Sites at Solid-Base Catalysts. 4th International Symposium Advanced Micro- and Mesoporous Materials 2011, Book of Abstracts, p. 110, Riviera Resort, Bulgaria, 6-9 September 2011.

[22] Čapek P., Veselý V., Kolafa J., Hejtmánek V., Brabec L.: Simulace transportu hmoty v replikách pórovitých látek pro účely odhadu jejich efektivních transportních vlastností. (Czech) Mass Transport Simulation in Replicas of Porous Material: Effective Transport Properties Estimation. 58. Konference

chemického a procesního inženýrství CHISA 2011, Sborník, 12 pp. full text on CD-ROM, p. 25 (B1.2), Srní, Šumava, Czech Republic, 24-27 October 2011.

[23] Kaštánek F., Sobek J., Kaštánek P., Šolcová O., Hájek M.: Dehalogenation of Polyhalogenated Compounds Dissolved in Organic Solvents with the Help of AOPs in a Two-Phase Solvent-Water System under the Influence of Ultrasound. 12th International Conference on Environmental Science and Technology CEST 2011, Proceedings, p. 114, Dodecanese, Rhodes Island, Greece, 8-10 September 2011.

[24] Morozová M., Klusoň P., Krýsa J., Veselý V., Dzik P., Šolcová O.: Thin TiO_2 Sol-Gel Layers Deposited by Three Various Methods. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1211-1213, Tatranské Matliare, Slovakia, 23-27 May 2011.

[25] Pohořelý M., Jeremiáš M., Kameníková P., Svoboda K., Skoblia S., Šyc M., Punčochář M.: Termické využití biomasy procesem parciální oxidace. (Czech) Biomass Termical Treatment by Partial Oxidation. 63. Zjazd chemikov, ChemZi 7(13), pp. 119-120, 2011, Tatranské Matliare, Vysoké Tatry, Slovakia, 5-9 September 2011.

[26] Poloncarzová M., Vejražka J., Veselý V., Izák P.: Effective Purification of Biogas by a Condensing-Liquid Membrane. 38th International Conference of Slovak Society of Chemical Engineering , p. 102, Tatranské Matliare, Slovakia, 23-27 May 2011.

[27] Svoboda K.: Kogenerace s využitím biomasy, vhodné výkony a možnosti efektivního využití tepla. (Czech) Biomass Based Cogeneration - Suitable Power Range and Possibilities of Effective Heat Utilization. 3. mezinárodní konference evropských manažerů pro energetiku, Praha, Czech Republic, 10-11 November 2011.

[28] Svoboda K., Pohořelý M., Jeremiáš M., Kameníková P., Hartman M., Skoblia S.: Fluidized Bed Oxyfuel ($CO_2 + O_2$) Gasification of Coal-Oil and Coal-Water-Oil Slurries. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1363-1375, Tatranské Matliare, Slovakia, 23-27 May 2011.

[29] Svoboda K., Pohořelý M., Kameníková P., Jeremiáš M., Skoblia S., Šyc M., Punčochář M.: Gasification of a Coal, Biomass, and a Coal-Biomass Mixture in a Fluidized Bed of Dolomite Particles by a Gas Containing Oxygen-CO_2 Mixtures. International Conference on Carbon Reduction Technologies CaReTECH 2011, Proceedings, p. 114-115, Polish Jurassic Highland (Orle Gniazdo), Poland, 19-22 September 2011.

[30] Svoboda K., Pohořelý M., Šyc M., Šulc J., Hartman M., Valeš V., Krček M.: Effects of Straw, Paper and Char Blending with Wood on Mechanical and Gasification Properties of Wood-Blend Pellets. 38th International Conference of Slovak Society of Chemical Engineering, p. 1022-1031, Tatranské Matliare, Slovakia, 23-27 May 2011.

[31] Šyc M, Pohořelý M., Jeremiáš M., Kameníková P., Svoboda K., Punčochář M.: Možnosti využití biomasy z fytoextrakce těžkých kovů. (Czech) The Possibilities of Using Biomass from Heavy Metals Fytoextraction. 63. Zjazd chemikov, ChemZi 7(13), p. 262, 2011, Tatranské Matliare, Vysoké Tatry, Slovakia, 5-9 September 2011.

[32] Šyc M., Pohořelý M., Jeremiáš M., Kameníková P., Punčochář M.: Distribution of Heavy Metals During Phytoextraction Crops Gasification and Combustion. (Eng) 1st Environment Asia International Conference on "Environmental Supporting in Food and Energy Security: Crisis and Opportunity", Proceedings, p.807-812, Bangkok, Thailand, 22-25 March 2011.

[33] Tukač V., Hanika J., Veselý V., Kovač D., Lederer J.: Simulace parciální oxidace biomasy. (Czech) Simulation of Biomass Partial Oxidation. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, pp. 173-180, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

[34] Tukač V., Hanika J., Veselý V., Kovač D., Lederer J.: Modelování parciální oxidace olejové suspenze biomasy. (Czech) Modeling of Partial Oxidation of Biomass Oil Suspension. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 56 (C2.6), Srní, Šumava, Czech Republic, 24-27 October 2011.

[35] Tukač V., Hanika J., Veselý V., Lederer J., Kovač D.: Simulation of Biomass Partial Oxidation. 1st International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH), Proceedings, Session 1, Poster 111, pp. 422-424, Noordwijkerhout, Netherlands, 29-31 July 2011.

[36] Veselý V., Hanika J., Lederer J., Nečesaný F., Kukačka J.: Tvorba a eliminace emisí PCDD/F při spalování odpadních plastů. (Czech) Formation and Elimination of Emissions of PCDD/F at Combustion of Waste Plastic Materials. 1st World Conference PETrA 2011 Pollution and Environment - Treatment of Air , Poster section, pp. 1-6 full text on CD-ROM, p. 1-6, Prague, Czech Republic, 17-20 May 2011.

Department of Aerosols and Laser Studies

HEAD
VLADIMÍR ŽDÍMAL

DEPUTY
RADEK FAJGAR

RESEARCH STAFF
IRENA BENEŠOVÁ ŠEVČÍKOVÁ, DAVID BRUS, VLADISLAV DŘÍNEK, JOSEF KUGLER, VALERI V. LEVDANSKI, PAVEL MORAVEC, JAKUB ONDRÁČEK, LUCIE ONDRÁČKOVÁ (DŽUMBOVÁ), DANA POKORNÁ, JOSEF POLA, JAROSLAV SCHWARZ, JIŘÍ SMOLÍK, DANIELA ŘIMNÁČOVÁ, TEREZA TRÁVNÍČKOVÁ, MARKÉTA URBANOVÁ, PETR VODIČKA
Part time: JAROSLAV KUPČÍK

PHD STUDENTS
VĚRA JANDOVÁ, MARTIN KOŠTEJN, OTAKAR MAKEŠ, LUDMILA MAŠKOVÁ (ANDĚLOVÁ), JAN PUŠMAN, LENKA ŠKRABALOVÁ, NADĚŽDA ZÍKOVÁ, LUBOŠ KRABÁČ

TECHNICAL STAFF
DARIA BARTLOVÁ

Fields of research

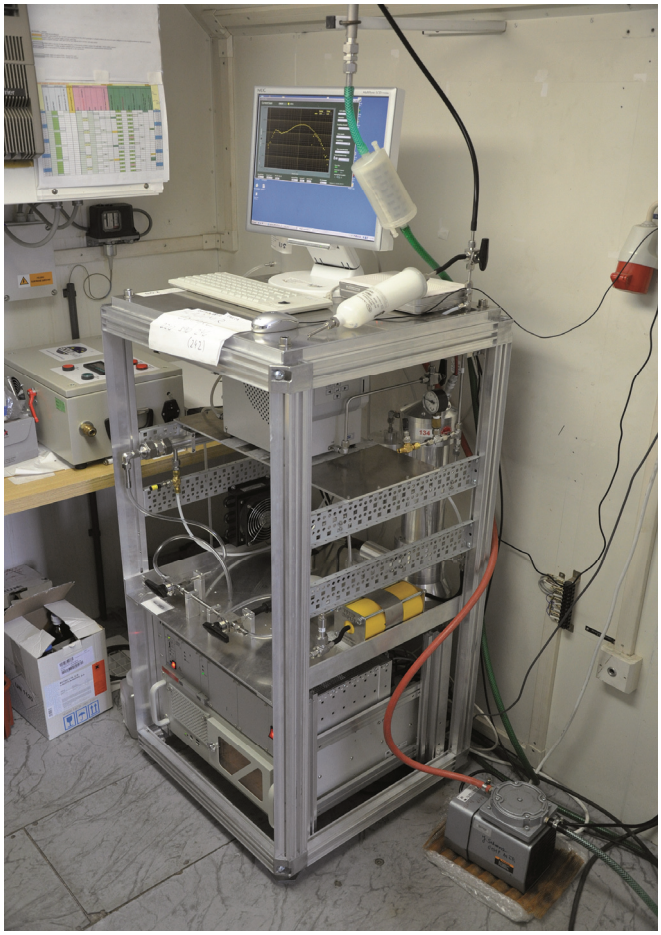
- Atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- Synthesis of nanoparticles *via* aerosol processes
- Heat and mass transfer in aerosol systems
- Interaction of aerosols with electromagnetic radiation
- Emissions sampling
- Nanoparticles and health
- Aerosol technology
- IR and UV laser induced chemistry
- Chemical vapor deposition of novel C-, Si- and Ge-based nanostructured materials
- IR laser-induced carbothermal reduction of oxides
- IR and UV laser photopolymerization in the gas phase
- UV laser chemical liquid deposition of metal nanosols and nanocomposites
- CVD of nanostructured objects (nanowires, nanoplatelets)
- IR and UV laser deposition of TiO_2-based materials
- IR and UV laser ablation for deposition of thin films

Research projects

European supersites for atmospheric aerosol research

(J. Schwarz, schwarz@icpf.cas.cz; supported by EC, 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. 1, 8, 18, 52, 53, 66, 67]



A photo of scanning mobility particle sizer measuring size distribution of particles at background site Košetice

Thermophysical properties of water in unexplored, technologically significant regions

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

This project focuses primarily on liquid water and solutions of selected salts below the freezing point (supercooled water), and water in nano-droplets. Existing hypotheses include the possibility of phase separation of supercooled water into two liquid phases below the second critical point. Density of supercooled water is only known at 0.1 MPa. Suggested measurements up to 100 MPa will provide first data. A new method and apparatus will be developed. The surface tension of supercooled water and a salt solution will be measured. The

surface tension of nano-droplets will be estimated from nucleation experiments. A range of theoretical approaches including phenomenological methods, simplified microscopic models, and molecular simulations, will be used with experimental data to obtain fundamental findings and engineering models. [Refs. 9, 10, 23, 32-41]

New ways to synthesize nanoparticles of various oxides

(V. Ždímal, zdimal@icpf.cas.cz; joint project with the ICT and Spolchemie a.s., supported by MIT, grant No. FR-TI1/548)

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. 27, 68]

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

(J. Schwarz, schwarz@icpf.cas.cz; joint project with Nuclear Physics Institute of the ASCR, v. v. i., supported by GACR, grant No. 205/09/2055)

The objectives of project can be summarized as follows: Atmospheric aerosol elemental composition on daily based samples will be 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 will be identified. Main source regions and their impact on regional air quality will be studied by combining the aerosol composition analysis with air mass transport history study. The obtained results will be compared with data available from 1990s to assess the impact of economical and structural changes in Central European economy on air pollution. [Refs. 21, 55-58, 61]

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

(V.V. Levdanski, valerij@icpf.cas.cz; supported by GA ASCR, grant No. IAA400720804)

The aim of the proposed 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. It is assumed to study the joint influence of size effects, electric charge and adsorbable foreign gases on formation of nanoparticles. Novel methods of the membrane purification of gases under influence of resonance radiation are assumed to be considered. The effect of radiation on mass transfer and storage of hydrogen in metallic nanoparticles will be investigated. The influence of electromagnetic radiation on coagulation, coalescence of nanoparticles and their deposition on a surface will be studied. [Refs. 9, 10, 23, 32-41]

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

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

All of the evidence from animal and human studies showed that there are risks associated with inhalation of nano-sized particles (NSP). The alveolar translocation of NSP is likely the pathway how NSP can be transposed from air to the blood vessels, and distributed throughout the body to organs. In spite of the fact that an extrapulmonary translocation is highly dependent on particle surface characteristics/chemistry, in addition to particle size, the study of transport of inhalated nano-particles Pb, Cd (elements, oxides), their allocations in organs, as well as study of toxicity these nanoparticles will be carry out with nanoparticles (10, 20 and 60 nm). The nonbiogenous elements (Cd, Pb) have been selected as products of

technological processes and due to their presence in ambient aerosol. The research will give us more information for a proper understanding of risks of technologies producing Cd and Pb nano-sized particles and ambient aerosol risk. [Refs. 6, 20, 50, 51, 60]

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

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

The aim of the project is to determine some properties of heterogeneous nuclei present in the superheated steam of steam turbines. In this project, the sampling device, coupled to advanced aerosol instrumentation (condensation particle counter, scanning mobility particle sizer), will be used to measure heterogeneous particles at selected power stations. To enable measurements of particles down to about 1 nm, a fast expansion chamber will be developed, enabling resolution of particle size by variable supersaturation. Collected data will serve as a basis for understanding the transport and the state of agglomeration of chemicals present in the steam circuit, for quantifying their effect on condensation, and, consequently, on the efficiency and reliability of steam turbines. [Refs. 9, 10, 23, 32-41]

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

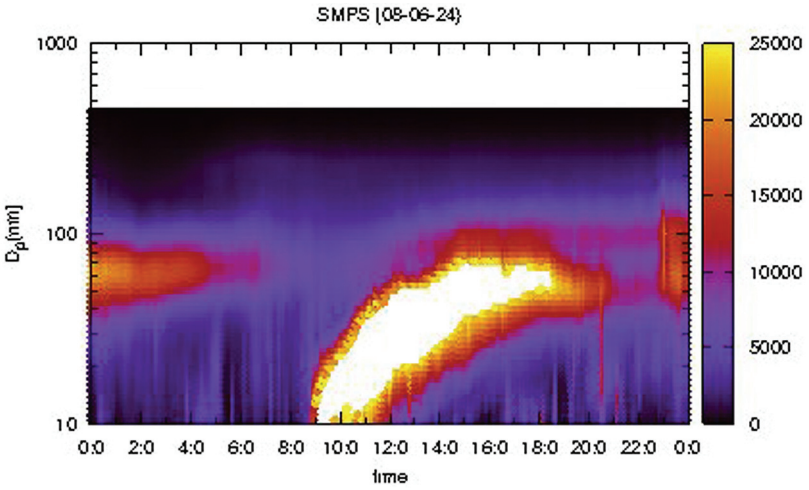
(J. Smolík, smolik@icpf.cas.cz; supported by the Ministry of Culture of the CR, project No. DF11P01OVV020)

The aims of the project are: a) development of evaluation methods for indoor air quality in libraries and archives, targeted at reduction of damages on library and archival collections caused by adverse effects of environment and b) gaining detailed knowledge of direct dependences between damage of library and archival collections and surrounding environment, leading to precautions reducing the adverse effects of deteriorated environment. [Refs. 11, 42, 43, 44, 59]

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

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

Advanced physical and chemical properties of Central European atmospheric aerosol at rural background and urban background sites will be studied in high time and size resolution. Parallel measurement of aerosol volatility will be carried out using a C-ToF-AMS equipped with a thermodenuder inlet, aerosol hygroscopicity using an HTDMA, and particle number size distribution using an SMPS. The information about aerosol particle density will be extracted from the SMPS and AMS. Hygroscopicity closure will be obtained from the combined HTDMA and AMS chemical composition data allowing to study the influence of organic aerosol on particles' hygroscopicity. The content of primary and secondary organic aerosol and the extent of aerosol ageing will be determined using AMS data at each site. In addition, at least a year-long time evolution of number size distributions obtained using the SMPS and OC/EC concentrations from the OC/EC analyzer will be delivered to the EBAS database, to be available for global atmospheric modeling groups [Refs. 13, 19, 22, 52-54, 56, 62-67].



Daily course of number and size of the new aerosol particles „banana“ type recorded by spectrometer SMPS

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

(J. Pola, pola@icpf.cas.cz; supported by GA ASCR, grant No. IAA400720619)

Megawatt KrF laser gas-phase photolysis of benzene and acetonitrile–benzene mixture was studied by using mass spectroscopy-gas chromatography and Fourier transform infrared spectroscopy for analysis of volatile products, and by Fourier transform infrared, Raman and X-ray photoelectron spectroscopy, electron microscopy and magnetization measurements for analyses of solid products deposited from the gas-phase. The results are consistent with carbonization of benzene and decomposition of non-absorbing acetonitrile in carbonizing benzene through collisions with excited benzene and/or its fragments. The solid products from benzene and acetonitrile-benzene mixture have large surface area and are characterized as nanomagnetic amorphous carbonaceous soot containing unsaturated C centers prone to oxidation. The nanosoot from acetonitrile-benzene mixture incorporates CN groups, confirms reactions of benzene fragments with CN radical and has a potential for modification by reactions at the CN bonds.

Pulsed infrared laser-irradiation of titanium monoxide leads to ablation and when carried out in gaseous benzene (1-5 Torr) to simultaneous dielectric breakdown of benzene into low molecular carbonaceous species which allow carbothermal reduction of ablated TiO_x particles and their protection by carbonaceous shell. The deposited particles are characterized by Fourier transform infrared Raman and X-ray photoelectron spectroscopy and by electron microscopy and shown to be stable towards oxidation in air. The reported process can find use in protection of gas-phase produced reactive nanoparticles by carbon phase. [Refs. 5, 15, 25, 26]

Laser approach to metal nanoalloys, its optimization & search for novel alloy nanostructures

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

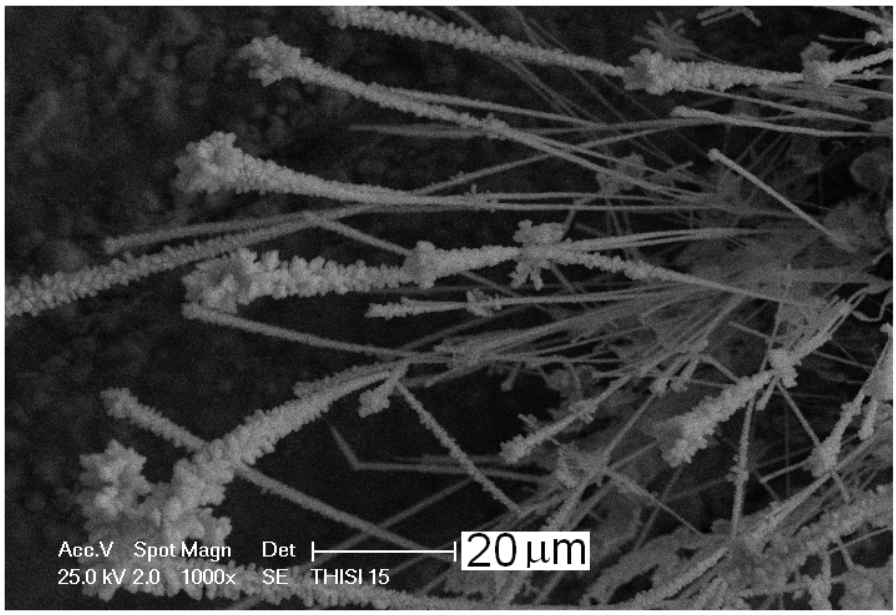
Pulsed IR laser irradiation of $SmCo_5$ alloy in vacuum and in adjacent dielectric breakdown (DB) of benzene has been examined as a tool for modifying phase and composition of this alloy and for suitability to serve as a laser deposition technique of Sm-Co nanoparticles and Sm-Co/C films. The composition of solid deposits was determined by FTIR, X-ray photoelectron and Raman spectroscopy and electron microscopy, and gas-phase chemical changes upon irradiation in gaseous benzene were analyzed by gas-chromatography

and FTIR and GC/MS spectroscopy. IR laser ablation in vacuum leads to deposition of amorphous $Sm_{1.00}$ $Co_{2.1\text{-}2.2}$ films containing uniformly dispersed Co_2Sm_5 nanocrystals and to formation of residual Sm_2Co_{17} target phase, both of which indicating disproportionation of $SmCo_5$ and Sm-enrichment of ablated particles. IR laser ablation in benzene results in formation of ultrafine powders consisting in fully amorphous $Sm_{1.00}Co_{4.2\text{-}4.6}$ nanoparticles embedded in amorphous hydrogenated carbonaceous phase and is in keeping with minor structural changes in ablated $SmCo_5$ particles. Both deposited materials are shown to differ in magnetic properties and the carbonaceous shell serves as a protection of Sm-Co nanobodies towards atmospheric oxidation. [Ref. 16]

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

(J. Pola, pola@icpf.cas.cz; supported by GACR, grant No. 203/09/0931)

UV laser photolysis of thiirane allows chemical vapor deposition of sulfur-containing solid which undergoes room-temperature reaction with copper and yields sub μm-sized amorphous filamentary $CuS/Cu_2S/C/H$ structures incorporating CuS and Cu_2S nanograins. Properties of these structures were examined by FTIR, Raman and X-ray photoelectron spectroscopies, X-ray diffraction and by electron microscopy. The results demonstrate the first example of reaction between solid sulfidizing reagent and copper at room temperature. [Ref. 17]

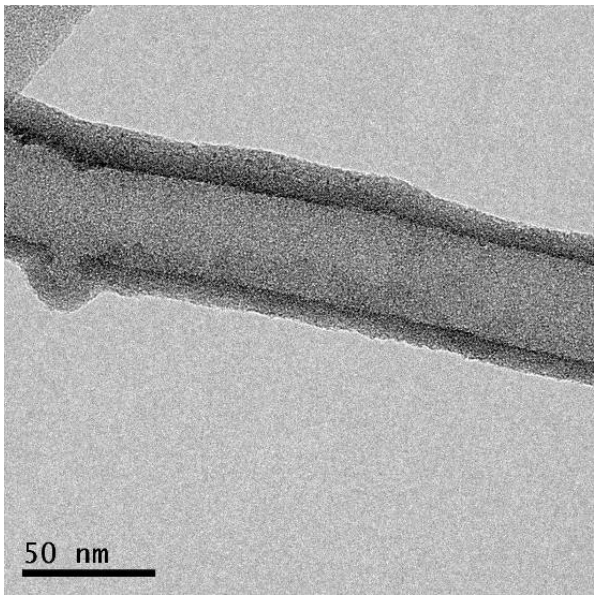


Laser deposited sub-μm-sized flower-like filamentary CuS_x features

Preparation of Si/O/C nanotubes using germanium nanowires as templates

(V. Dřínek, drinek@icpf.cas.cz; supported by GACR, grant No. 203/09/1088)

Low Pressure CVD of hexamethyldigermane Ge_2Me_6 and tetramethyldisilazane $(SiMe_2H)_2NH$ resulted in the growth of Ge nanowires wrapped in Si/O/C material. Nitrogen in the grown structure was replaced by oxygen due to its traces in the vacuum chamber. Subsequent annealing to 850 °C under vacuum lead to evaporation of germanium so that silicon oxycarbide nanotubes were formed. The nanotubes diameter was up to 80 nm, the length several microns. The nanotubes of such kind are very promising in the chemical catalysis. [Refs. 7, 14, 30, 31]



High resolution TEM image of the Si/O/C nanotube

Excimer laser-induced CVD of carbon encapsulated cobalt nanoparticles

(R. Fajgar, fajgar@icpf.cas.cz; supported by GACR, grant No. 203/09/1117)

Decomposition of acetylene/$Co(CO)_3(NO)$ mixtures induced by excimer ArF laser pulses is an efficient technique for preparation of amorphous cobalt nanoparticles encapsulated in carbon. Vacuum annealing up to 1170 K leads to structural changes both in the metal core and carbon shells. The cobalt core crystallizes in a face-centered cubic (β) form as revealed by X-ray and electron diffraction techniques and carbon affords graphite outer part. Properties of the Co(core) - carbon(shell) nanocomposites were examined by spectroscopy and microscopy techniques. Magnetization studies revealed superparamagnetic behaviour of the as-prepared amorphous deposit up to 150 K while annealed samples are ferromagnetic due to the size of the cobalt cores larger than 20 nm.

Excimer laser deposition and characterization of cerium doped TiO_2

(R. Fajgar, fajgar@icpf.cas.cz; supported by GACR, grant No. 203/09/1117)

Thin layers of Ti/Ce/O photocatalyst were deposited by ArF excimer laser ablation of oxide targets. Pellets of TiO_2 and CeO_2 were alternately irradiated by laser beam (193 nm) with fluence 6.0 $J.cm^{-2}$. Non-stoichiometric titanium oxides with 1-10% cerium were deposited on glass, quartz and tantalum substrates as thin multilayers and characterized by spectroscopic, microscopic and diffraction techniques. The as-prepared films with thickness 150 nm possess good adhesion to substrates and very poor degree of crystallization, as demonstrated by broad diffusion rings in selected area electron diffraction (SAED) pattern. Heating of the oxides in air (450 ^{o}C / 2h) leads to crystallization of the deposited material and its superhydrophylic behaviour. The nanocrystalline film shows the discrete SAED rings of anatase TiO_2 and cubic CeO_2 nanocrystallites. The Raman spectrum of the annealed deposit revealed bands attributable to anatase form of TiO_2 and cubic CeO_2. UV-VIS spectroscopy demonstrates successful shift of the absorption edge to the visible region. [Ref. 29, 47]

International co-operations

Division of Nuclear Physics, Department of Physics, Lund University, Lund, Sweden
Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
Ghent University, Institute for Nuclear Sciences, Ghent, Belgium: OC/EC in urban and suburban PM10 aerosol in Prague, Hygroscopic properties of urban and suburban carbonaceous aerosols
Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan
Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, Switzerland
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behaviour
Southern Illinois University Carbondale, Carbondale, IL, USA: Friction materials based on polymer matrix containing metals and their impact on environment
Technical University of Crete, Chania, Greece: Aerosols in the environment
University of Helsinki, Division of Atmospheric Sciences, Helsinki, Finland
Tampere University of Technology, Tampere, Finland: Synthesis and characterization of nanosized metal/ceramic particles
University of Eastern Finland, Kuopio, Finland: Novel aerosol generation processes focused on medical treatment and nanotechnology
Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodź, Poland: UV laser-induced cross-linking of polysiloxanes
Faculty of Technology and Metallurgy, University of St. Cyril & Methodius, Skopje, Republic of Macedonia: Novel preparation and photocatalytic study of titania-based catalysts
Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of nanosized metal chalcogenides and polycarbosilathianes
King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia: Laser degradation of contaminants in fuel oils
National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania: Laser-induced CVD of Fe/polymer nanocomposites
National Institute of Advanced Industrial Research and Technology, Tsukuba, Japan: Laser control of organic reactions
POLYMAT, Institute for Polymer Materials, San Sebastian, Spain: Laser ablation of graphene-based composites
University of Crete, Heraklion, Greece: Laser induced chemical vapour deposition of polycarbosilathianes

Visits abroad

D. Brus: Finnish Meteorological Institute, Helsinki, Finland (12 months)
L. Škrabalová: Finnish Meteorological Institute, Helsinki, Finland (1 month)
V. Jandová: Instituto de Estructura de la Materia, CSIC, Madrid, Spain (3 months)

Visitors

T. Hussein, University of Helsinki, Helsinki, Finland
V. Nororos, University of Helsinki, Helsinki, Finland
J. Blazevska-Gilev, University of St. Cyril & Methodius, Skopje, R. Macedonia
Nguyen Thanh Danh, Institute of Chemical Technology, VAST, Ho Chi Minh City, Vietnam

Ta Anh Tuan, HCM City Institute of Physics, VAST, Ho Chi Minh City, Vietnam
Radmila Tomovska, POLYMAT, Institute for Polymer Materials, San Sebastian, Spain
Xiaofeng Chang: Nanking University of Aeronautics and Astronautics, Nanking, China

Teaching

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

Publications

Original papers

[1] Asmi A., Wiedensohler A., Laj P., Fjaeraa A.-M., Sellegri K., Birmili W., Weingartner E., Baltensperger U., Ždímal V., Zíková N., Putaud J.-P., Marinoni A, Tunved P., Hansson H.-C., Fiebig M., Kivekäs N., Lihavainen H., Asmi E., Ulevicius V., Aalto P.P., Swietlicki E., Kristensson A., Mihalopoulos N., Kalivitis N., Kalapov I., Kiss G., de Leeuw G., Henzing B., Harrison R.M., Beddows D., O'Dowd C., Jennings S.G., Flentje H., Weinhold K., Meinhardt F., Ries L., and Kulmala M.: Number Size Distributions and Seasonality of Submicron Particles in Europe 2008-2009. *Atmos. Chem. Phys.* 11(11), 5505-5538 (2011).

[2] Brus D., Neitola K., Hyvärinen A.-P., Petäjä T., Vanhanen J., Sipilä M., Paasonen P., Kulmala M., Lihavainen H.: Homogenous Nucleation of Sulfuric Acid and Water at Close to Atmospherically Relevant Conditions. *Atmos. Chem. Phys.* 11(11), 5277–5287 (2011).

[3] Hyvärinen A., Raatikainen T., Brus D., Komppula M., Panwar T.S., Hooda R.K., Sharma V.P., Lihavainen H.: Effect of the Summer Monsoon on Aerosols at Two Measurement Stations in Northern India – Part 1: PM and BC Concentrations. *Atmos. Chem. Phys.* 11(16), 8271-8282 (2011).

[4] Hyvärinen A.-P., Raatikainen T., Komppula M., Mielonen T., Sundström A.-M., Brus D., Panwar T.S., Hooda R.K., Sharma V.P., de Leeuw G., Lihavainen H.: Effect of the Summer Monsoon on Aerosols at Two Measurement Stations in Northern India – Part 2: Physical and Optical Properties. *Atmos. Chem. Phys.* 11(16), 8283-8294 (2011).

[5] Jandová V., Bastl Z., Šubrt J., Pola J.: IR Laser-Produced Carbon-Phase Shield to Oxidation of Nanosized Titanium Monoxide. *J. Anal. Appl. Pyrol.* 92(2), 287-291 (2011).

[6] Kukutschová J., Moravec P., Tomášek V., Matějka V., Smolík J., Schwarz J., Seidlerová J., Šafářová K., Filip P.: On Airborne Nano/Micro-Sized Particles Released from Low-Metallic Automotive Brakes. *Environ. Pollut.* 159(4), 998-1006 (2011).

[7] Křenek T., Fajgar R., Medlín R., Klementová M., Novotný F., Dřínek V.: Fabrication of Cu_xGe_y Nanoplatelets. *J. Nanosci. Nanotechnol.* 11(9), 8279-8283 (2011).

[8] Kulmala M., Asmi A., Lappalainen H.K., Baltensperger U., Brenguier J.L., Facchini M.C., Hansson H.-C., Hov Q., O'Dowd C.D., Pöschl U., Wiedensohler A., Boers R., Boucher O., de Leeuw G., Denier van der Gon H.A.C., Feichter J., Krejci R., Laj P., Lihavainen H., Lohmann U., McFiggans G., Mentel T., Pilinis C., Riipinen I., Schulz M., Stohl A., Swietlicki E., Vignati E., Alves C., Amann M., Ammann M., Arabas S., Artaxo P., Baars H., Beddows D.C.S., Bergström R., Beukes J.P., Bilde M., Burkhart J.F., Canonaco F., Clegg S.L., Coe H., Crumeyrolle S., D'Anna B., Decesari S., Gilardoni S., Fischer M., Fjaeraa A.M., Fountoukis C., George C., Gomes L., Halloran P., Hamburger T., Harrison R.M., Herrmann H., Hoffmann T., Hoose C., Hu M., Hyvärinen A., Hörrak U., Iinuma Y., Iversen T., Josipovic M., Kanakidou M., Kiendler-Scharr A., Kirkevåg A., Kiss G., Klimont Z., Kolmonen P., Komppula M., Kristjánsson J.E., Laakso L., Laaksonen A., Labonnote L., Lanz V.A., Lehtinen K.E.J., Rizzo L.V., Makkonen R., Manninen H.E., McMeeking G., Merikanto J., Minikin A., Mirme S., Morgan W.T.,

Nemitz E., O'Donnell D., Panwar T.S., Pawlowska H., Petzold A., Pienaar J.J., Pio C., Plass-Duelmer C., Prévôt A.S.H., Pryor S., Reddington C.L., Roberts G., Rosenfeld D., Schwarz J., Seland Ø., Sellegri K., Shen X.J., Shiraiwa M., Siebert H., Sierau B., Simpson D., Sun J.Y., Topping D., Tunved P., Vaattovaara P., Vakkari V., Veefkind J.P., Visschedijk A., Vuollekoski H., Vuolo R., Wehner B., Wildt J., Woodward S., Worsnop D.R., van Zadelhoff G.-J., Zardini A.A., Zhang K., van Zyl P.G., Kerminen V.-M., Carslaw K.S., and Pandis S.N.: General Overview: European Integrated project on Aerosol Cloud Climate and Air Quality Interactions (EUCAARI) – Integrating Aerosol Research from Nano to Global Scales. *Atmos. Chem. Phys.* 11(24), 13061–13143 (2011).

[9] Levdansky V.V., Dragun V.L., Smolík J., Ždímal V.: Zakhvat molekul para nanochastitsami (klasterami) i problema gomogennoi nukleatsii. (Russ) . *Vestci Nat. Ak. Nauk Belarusi, Ser. Fyz.-Tekh. Navuk* 3, 54-58 (2011).

[10] Levdansky V.V., Smolík J., Ždímal V.: Vliyanie razmernykh effektov na protsessy nukleatsii v kondensirovannoi faze. (Russ) . *Inzh.-Fyz. Zh.* [*J. Eng. Phys. Thermophys.* 84(3), 574-578, 2011] 84(3), 531-534 (2011).

[11] López-Aparicio S., Smolík J., Mašková L., Součková M., Grøntoft T., Ondráčková L., Stankiewicz J.: Relationship of Indoor and Outdoor Air Pollutants in a Naturally Ventilated Historical Building Envelope. *Build. Environ.* 46(7), 1460-1468 (2011).

[12] Moravec P., Smolík J., Keskinen H., Mäkelä J.M., Bakardjieva S., Levdansky V.V.: NiO_x Nanoparticle Synthesis by Chemical Vapor Deposition from Nickel Acetylacetonate. *Mater. Sci. Appl.* 2, 258-264 (2011).

[13] Ondráček J., Schwarz J., Ždímal V., Andělová L., Vodička P., Bízek V., Tsai C.-J., Chen S.-C., Smolík J.: Contribution of the Road Traffic to Air Pollution in the Prague City (Busy Speedway and Suburban Crossroads). *Atmos. Environ.* 45(29), 5090-5100 (2011).

[14] Palatinus L., Klementová M., Dřínek V., Jarošová M., Petříček V.: An Incommensura-tely Modulated Structure of η^0-Phase of $Cu_{3+x}Si$ Determined by Quantitative Electron Diffraction Tomography. *Inorg. Chem.* 50(8), 3743-3751 (2011).

[15] Pola J., Ouchi A., Maryško M., Vorlíček V., Šubrt J., Bakardjieva S., Bastl Z.: UV Laser Photodeposition of Nanomagnetic Soot from Gaseous Benzene and Acetonitrile-Benzene Mixture. *J. Photochem Photobiol., A: Chem.* 220(2-3), 188-194 (2011).

[16] Pola J., Pokorná D., Maryško M., Bastl Z., Šubrt J., Bakardjieva S., Bezdička P., Gondal M.A., Masoudi H.M.: IR Laser Deposition: Co_2Sm_5 Nanocrystals in Amorphous Sm-Co Phase and Amorphous Sm-Co Nanobodies in Carbonaceous Phase. *J. Photochem. Photobiol., A: Chem.* 223(2-3), 132-139 (2011).

[17] Pola J., Urbanová M., Pokorná D., Bastl Z., Bakardjieva S., Šubrt Š., Bezdička P.: Laser Photodeposition of Sulfur and Room-Temperature Solid-State Reaction with Copper. *J. Photochem. Photobiol., A: Chem.* 219(1), 109-114 (2011).

[18] Reddington C.L., Carslaw K.S., Spracklen D.V., Frontoso M.G., Collins L., Merikanto J., Minikin A., Hamburger T., Coe H., Kulmala M., Aalto P., Flentje H., Plass-Dülmer C., Birmili W., Wiedensohler A., Wehner B., Tuch T., Sonntag A., O'Dowd C.D., Jennings S.G., Dupuy R., Baltensperger U., Weingartner E., Hansson H.-C., Tunved P., Laj P., Sellegri K., Boulon J., Putaud J.-P., Gruening C., Swietlicki E., Roldin P., Henzing J.S., Moerman M., Mihalopoulos N., Kouvarakis G., Ždímal V., Zíková N., Marinoni A., Bonasoni P., and Duchi R.: Primary Versus Secondary Contributions to Particle Number Concentrations in the European Boundary Layer. *Atmos. Chem. Phys.* 11(23), 12007-12036 (2011).

[19] Řimnáčová D., Ždímal V., Schwarz J., Smolík J., Řimnáč M.: Atmospheric Aerosols in Suburb of Prague: The Dynamics of Particle Size Distributions. *Atmos. Res.* 101(3), 539-552 (2011).

[20] Smolík J., Ondráčková L., Maršíková J.: Koncentrace aerosolových částic v zubní ordinaci. (Czech) Aerosol Particle Concentration in a Dental Office. *Chem. Listy* 105(5), 371-374 (2011).

[21] Štefancová L., Schwarz J., Mäkelä T., Hillamo R., Smolík J.: Comprehensive Characterization of Original 10-stage and 7-stage Modified Berner Type Impactors. *Aerosol Sci. Technol.* 45(1), 88-100 (2011).

[22] Ždímal V., Smolík J., Eleftheriadis K., Wagner Z., Housiadas Ch., Mihalopoulos N., Mikuška P., Večeřa Z., Kopanakis I., Lazaridis M,.: Dynamics of Atmospheric Aerosol Number Size Distributions in the Eastern Mediterranean During the "SUB-AERO" Project. *Water Air Soil Pollut.* 214(1-4), 133-146 (2011).

Chapters in books

[23] Levdansky V.V., Dragun V.L., Ždímal V.: Isparenie zhidkosti iz nanorazmernogo kapillyara v prisutstvii postoronnego adsorbiruyuschegosya gaza. (Russ) . In: *Teplo- i Massoperenos - 2011*. (Dragun V.L., Ed.), p. 95-97, Institut teplo- i massoobmena A.V. Lykova, Minsk 2011.

Patents

[24] Gondal M.A., Pola J., Yamani Z. H., Masoudi H. M., Al-Arfaj A.R.A.: Laser-Based Method for Removal of Sulfur (DMDBT) in Hydrocarbon Fuels. *U.S. Pat. No. 7871501*. Applied: 06.11.15, Patented: 11.01.18.

International conferences

[25] Blazevska-Gilev J., Pola J.: Laser Ablative Modification of Poly(Ethylene-co-Acrylic Acid) Zinc Salt-Sodium Metasilicate. 2nd International Congress Engineering, Ecology and Materials in the Processing Industry, Proceedings, p. 563-568, Jahorina, Bosna a Hercegovina, 9-11 March 2011.

[26] Blazevska-Gilev J., Pola J.: Pulsed IR Laser Ablation of Poly(Ethylene-co-Acrylic Acid) Zinc Salt. 2nd International Congress Engineering, Ecology and Materials in the Processing Industry, Proceedings, p. 557-562, Jahorina, Bosna a Hercegovina, 9-11 March 2011.

[27] Brožek V., Mastný L., Moravec P., Neufuss K., Ondráček J., Ždímal V.: Procesy vzniku nanočástic v proudu nízkoteplotního plazmatu. (Czech) Processes of Nanoparticle Formation in Low Temperature Plasma. 58. Konference chemického a procesního inženýrství CHISA 2011, Sborník, p. 170 (V43), Srní, Šumava, Czech Republic, 24-27 October 2011.

[28] Brus D., Neitola K., Petäjä T., Lihavainen H.: Diffusion Coefficient Measurements of Sulphuric Acid in Air. European Aerosol Conference EAC 2011, Book of Abstracts, p. 456 (4P54), Manchester, Great Britain, 4-9 September 2011.

[29] Fajgar R., Dřínek V., Kupčík J., Šubrt J., Murafa N.: Excimer Laser Deposition and Characterization of Cerium Doped TiO_2. EuroCVD 18, Conference Programme and Abstracts, p. 131, Kinsale, Co. Cork, Ireland, 4-9 September 2011.

[30] Krabáč L., Dřínek V., Fajgar R., Klementová M.: Preparation of Si/N Based Nanotubes Using Germanium Nanowires as Template. EuroCVD 18, Conference Programme and Abstracts, p. 129, Kinsale, Co. Cork, Ireland, 4-9 September 2011.

[31] Křenek T., Dřínek V., Fajgar R., Medlín R., Klementová M.: Low Pressure Chemical Vapor Deposition of Ge_2Me_6 + $SnMe_4$ Mixture for Nanoplatelet Formation. EuroCVD 18, Conference Programme and Abstracts, p. 146, Kinsale, Co. Cork, Ireland, 4-9 September 2011.

[32] Levdansky V.V., Dragun V.L., Ždímal V., Moravec P.: Vliyanie razmera nanochastits na protekayuschie v nikh khimicheskie reaktsii. (Russ) . VI Mezhdunarodnoe simpozium "Fullereny i nanostruktury v kondensirovannykh sredakh" , Sbornik nauchnych statei, p. 314-317, Minsk, Belarus, 14-17 June 2011.

[33] Levdansky V.V., Smolík J., Ždímal V.: Size Effects in Heterogeneous Systems with Nanoscale Particles. E-MRS 2011 Spring Meeting IUMRS ICAM 2011 & E-MRS / MRS Bilateral Conference on Energy , Symposium C, p. PC3 16, Nice, France, 9-13 May 2011.

[34] Levdansky V.V., Smolík J., Ždímal V.: Influence of Size Effects on Growth Rate of Si Nanowhiskers. The International Conference on Physics, Chemistry and Application of Nanostructures "Nanomeeting 2011" , Reviews and Short Notes, p. 162-164, Minsk, Belarus, 24-27 May 2011.

[35] Levdansky V.V., Smolík J., Ždímal V.: Size Effects in Physicochemical Processes in Heterogeneous Systems with Nanoscale Objects. 15th Research Workshop Nucleation Theory and Applications, Third Announcement, Dubna, Russia, 1-30 April 2011.

[36] Levdansky V.V., Smolík J., Ždímal V.: Effect of Adsorption of Foreign Gases on Evaporation of Liquid from Nanoscale Capillaries. 4th International Symposium Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 112, Riviera Resort, Bulgaria, 6-9 September 2011.

[37] Levdansky V.V., Smolík J., Ždímal V.: Light-Induced Physicochemical Prcesses in Heterogeneous Systems with Nanoscale Objects. 19th International Conference on Advanced Laser Technologies - ALT'11, Book of Abstracts, p. 130-131, Golden Sands, Bulgaria, 3-8 September 2011.

[38] Levdansky V.V., Smolík J., Ždímal V.: Effect on Foreign Adsorbable Gases on Phase Transitions on Surface of Nanoscale Objects. 8th Liquid Matter Conference, Poster Abstracts, p. 25 (P6.25), Wien, Austria, 6-10 September 2011.

[39] Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Size Effect in Homogeneous Nucleation in Nanoscale Particles. European Aerosol Conference EAC 2011, Book of Abstracts, p. 562 (4P55), Manchester, Great Britain, 4-9 September 2011.

[40] Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Size-Dependent Rate Constant of Chemical Reactions in Nanoscale Particles. XII. Výroční konference České aerosolové společnosti, Sborník, p. 39-40, Čejkovice, Czech Republic, 3-4 November 2011.

[41] Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Influence of Size Effects on Homogeneous Nucleation Inside Nanoparticles. XII. Výroční konference České aerosolové společnosti, Sborník, p. 45-46, Čejkovice, Czech Republic, 3-4 November 2011.

[42] Mašková L., Smolík J., Ondráček J., Ohlídalová M.: Aerosol Particles in the Indoor Environment of the National Museum of the Czech Republic. European Aerosol Conference EAC 2011, Book of Abstracts, p. L12, Manchester, Great Britain, 3-9 September 2011.

[43] Mašková L., Smolík J., Ondráček J., Ohlídalová M.: Aerosolové částice ve vnitřním prostředí Národního muzea. (Czech) Aerosol Particles in the Indoor Environment of the National Museum. XII. Výroční konference České aerosolové společnosti, Sborník, p. 17-18, Čejkovice, Czech Republic, 3-4 November 2011.

[44] Mašková L., Smolík J., Ondráček J., Ondráčková L., López-Aparicio S.: Relationship of Indoor and Outdoor PM and Gaseous Pollutants in the National Library in Prague. European Aerosol Conference EAC 2011, Book of Abstracts, p. 102 (8P53), Manchester, Great Britain, 3-9 September 2011.

[45] Matějová L., Fajgar R., Matěj Z., Maléterová Y., Šolcová O.: Metal Oxide Aerogel. 2nd Nanomaterials and Nanotechnology Meeting Nano Ostrava 2011, Book of Abstracts, p. 11(OP-5), Ostrava, Czech Republic, 27-29 April 2011.

[46] Matějová L., Matěj Z., Fajgar R., Schneider P., Šolcová O.: Highly-Porous Metal Oxide Aerogels; Preparation and Characterization. 9th International Symposium on Characterization of Porous Solids - COPS 9, Book of Abstracts, p. 181, Dresden, Germany, 5-8 June 2011.

[47] Matějová L., Matěj Z., Fajgar R., Šolcová O.: Role of Subcritical Water Extraction in Crystallization of Highly-Porous Titania, Titania-Zirconia and Titania-Ceria Aerogels. 12th Conference of the European Ceramic Society ECerS XII, Poster Session II, p. 72 (2132), Stockholm, Sweden, 19-23 June 2011.

[48] Matějová L., Matěj Z., Fajgar R., Šolcová O.: Role of Subcritical Drying in Preparation of Crystalline Metal Oxides Aerogels. 4th International Symposium Advanced Micro- and Mesoporous Materials 2011, Book of Abstracts, p. 72, Riviera Resort, Bulgaria, 6-9 September 2011.

[49] Matějová L., Šnajdaufová H,, Matějková M., Fajgar R., Matěj Z., Šolcová O.: Optimization of Pressurized Fluid Extraction for Preparation of Metal Oxide Nanostructures. 38th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1207-1210, Tatranské Matliare, Slovakia, 23-27 May 2011.

[50] Moravec P., Smolík J., Bakardjieva S., Levdansky V.V.: Binary CoO_x/SiO_2 Nanoparticle Synthesis. European Aerosol Conference EAC 2011, Book of Abstracts, p. 972 (4P157), Manchester, Great Britain, 4-9 September 2011.

[51] Moravec P., Smolík J., Bakardjieva S., Levdansky V.V.: Generation of Binary CoO_x/SiO_2 Nanoparticles from Organocompound Precursors. XII. Výroční konference České aerosolové společnosti, Sborník, p. 85-88, Čejkovice, Czech Republic, 3-4 November 2011.

[52] Ondráček J., Vodička P.: Long Time Measurement of Aerosol Hydroscopicity at Košetice Backround Station. XII. Výroční konference České aerosolové společnosti, Sborník, p. 79-84, Čejkovice, Czech Republic, 3-4 November 2011.

[53] Ondráček J., Vodička P., Ždímal V., Schwarz J., Smolík J.: Hygroscopicity of Aerosol Particles at Kosetice Background Station (Czech Republic) Using the HTDMA System. European Aerosol Conference EAC 2011, Book of Abstracts, p. 933 (4P235), Manchester, Great Britain, 4-9 September 2011.

[54] Ondráček J., Ždímal V., Schwarz J., Bízek V., Smolík J.: Influence of the Road Traffic Intensity on Air Pollution in the Prague. European Aerosol Conference EAC 2011, Book of Abstracts, p. 932 (8P228), Manchester, Great Britain, 4-9 September 2011.

[55] Schwarz J.: The Ionic Composition of PM2.5 at a Rural Background Site in Central Europe on Daily Basis. European Aerosol Conference EAC 2011, Book of Abstracts, p. 900 (4P307), Manchester, Great Britain, 4-9 September 2011.

[56] Schwarz J., Havránek V.: Chemical Composition of PM2.5 at Rural Backround Site Košetice. XII. Výroční konference České aerosolové společnosti, Sborník, p. 37-38, Čejkovice, Czech Republic, 3-4 November 2011.

[57] Schwarz J., Karban J., Chalupníčková E., Pokorný R., Novák J., Smolík J.: The Influence of Biomass Burning on PM2.5 at Urban and Rural Background Sites in the Czech Republic. European Aerosol Conference EAC 2011, Book of Abstracts, p. 899 (4P306), Manchester, Great Britain, 4-9 September 2011.

[58] Schwarz J., Vodička P.: Two Years Experience with Two Sunset Semi-Online Field OC/EC Analyzers Running Side by Side. 10th International Conference on Carbonaceous Particles in the Atmosphere, Abstract Book, p. 125 (E22), Vídeň, Austria, 26-29 June 2011.

[59] Smolík J., Mašková L., Zíková N., Ondráček J.: Deposition of Aerosol Particles on Filter Surfaces. XII. Výroční konference České aerosolové společnosti, Sborník, pp. 19-24, Čejkovice, Czech Republic, 3-4 November 2011.

[60] Večeřa Z., Mikuška P., Dočekal B., Vojta Š., Míšek I., Moravec P., Smolík J.: Unique Exposure System for the Whole Body Inhalation Experiments with Small Animals . 3. ročník mezinárodní konference NANOCON 2011, Sborník, p. 107, Brno, Czech Republic, 21-23 September 2011.

[61] Vodička P., Schwarz J.: EC/OC and OC Fractions from Two Czech Sites in Parallel and Their Relationships with Meterology. 10th International Conference on Carbonaceous Particles in the Atmosphere, Posters, p. 70, Vienna, Austria, 26-29 June 2011.

[62] Vodička P., Schwarz J.: Diurnal Trends of Carbonaceous Aerosols at Prague Suburban Station during Different Seasons. XII. Výroční konference České aerosolové společnosti, Sborník, p. 51-54, Čejkovice, Czech Republic, 3-4 November 2011.

[63] Wagner Z., Fridrich M., Schwarz J., Ždímal V., Váňa M.: Measurement and Analysis of Near Real Time Data on Particle Size Distribution in Atmospheric Aerosol. 36th International Invention Show (gold medal awarded), Katalog, p. 130, Zagreb, Croatia, 9-12 November 2011.

[64] Wagner Z., Fridrich M., Schwarz J., Ždímal V.: Zpracování hromadných dat distribuce velikosti aerosolových částic v reálném čase a jejich prezentace v evropských i celosvětových databázích. (Czech) Analysis of Near Real Time Data on Particle Size Distribution in Atmospheric Aerosol and Their

Presentation in International Databases. TeXperience 2011 (4.ročník) a Stakan 2011 (6.ročník), Kniha abstraktů, pp. 33-34, Železná Ruda, Czech Republic, 20 September - 2 October 2011.

[65] Zíková N., Ždímal V.: Connection of Atmospheric Stability and Aerosol and Gaseous Polutants Concentration. Goldschmidt 2011, *Mineralogical Magazine* 75 (3), 2286, 2011, Prague, Czech Republic, 14-19 August 2011.

[66] Zíková N., Ždímal V.: SMS spektra při různých meteorologických podmínkách. (Czech) SMPS Spectra during Various Meteorological Conditions. XII. Výroční konference České aerosolové společnosti, Sborník, pp. 75-78, Čejkovice, Czech Republic, 3-4 November 2011.

[67] Zíková N., Ždímal V., Smolík J.: SMPS Spectra Under Various Meteorological Conditions. European Aerosol Conference EAC 2011, Book of Abstracts, p. 129 (4P213), Manchester, Great Britain, 4-9 September 2011.

[68] Ždímal V., Moravec P., Doležal B., Brožek V., Neufuss K.: Aerosolové nanočástice vznikající při plazmové depozici. (Czech) Aerosol Nanoparticles Formed during Plasma Deposition. 20. Chemicko-technologická konference s mezinárodní účastí APROCHEM 2011, Sborník přednášek, pp. 591-598, Kouty nad Desnou, Czech Republic, 11-13 April 2011.

INTERNATIONAL ADVISORY BOARD OF ICPF

VLADIMÍR BÁLEŠ, Slovak University of Technology, Bratislava, Slovakia
LIANG-SHIN FAN, Ohio State University, Columbus, OH, USA
ANASTASIOS J. KARABELAS, Aristotle University of Thessaloniki, Greece
VALERII A. KIRILLOV, Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
JAN C. M. MARIJNISSEN, Delft University of Technology, Delft, Netherlands
ALVIN W. NIENOW, University of Birmingham, Birmingham, UK
AKIHIKO OUCHI, National Insitute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan
RYSZARD POHORECKI, Warsaw University of Technology, Warszaw, Poland
TAPIO O. SALMI, Åbo Akademi University, Åbo-Turku, Finland
SILVIO SICARDI, Polytechnic University of Turin, Turin, Italy
PHILIPPE UNGERER, French Institute of Petroleum, Rueil-Malmaison, France
GABRIEL WILD, ENSIC CNRS, Nancy, France

MEMBERSHIPS IN EDITORIAL BOARDS

G. BOGDANIĆ: "Journal of Macromolecular Science, Part A. Pure and Applied Chemistry"
G. BOGDANIĆ: "Kemija u Industriji"
G. BOGDANIĆ: "Polimeri"
J. ČERMÁK: "Chemical Papers"
J. DRAHOŠ: "Chemical Engineering Research and Design"
J. DRAHOŠ: "Clean Products and Processes"
J. DRAHOŠ: "International Journal of Multiphase Flow"
J. HANIKA: "Hemijska Industrija/Chemical Industry"
J. HANIKA: "Chemical Industry & Chemical Engineering Quarterly"
J. HANIKA: "Chemical Papers"
J. HETFLEJŠ: "Chemické Listy"
K. JEŘÁBEK: "Reactive and Functional Polymers"
V. JIŘIČNÝ: "South African Journal of Chemical Engineering"
I. NEZBEDA: "International Journal of Liquid State Sciences"
I. NEZBEDA: "Molecular Physics"
J. POLA: "Materials Science : An Indian Journal"
J. POLA: "Macromolecules : An Indian Journal"
J. SMOLÍK: "Aerosol and Air Quality Research"
I. WICHTERLE: "Kemija u Industriji"

Memberships in International Scientific Bodies

K. AIM: International Steering Committee, 25th European Symposium on Applied Thermo-dynamics (ESAT 2011), Saint Petersburg, Russia, 24-27 June, 2011 (http://onlinereg.ru/site.php?go=145&page=2401&lang=ENG)

K. AIM: Moderator, European Science Foundation, Member Organisation Forum on Science Foresight for Joint Strategy Development, 2nd Workshop, Madrid, Spain, 19-20 January 2011 (http://www.esf.org/activities/mo-fora/science-foresight-for-joint-strategy-development.html)

J. ČERMÁK: International Advisory Board, European Association for Chemical and Molecular Sciences - Division of Organometallic Chemistry, XIX EuCHEMS Conference on Organometallic Chemistry (EuCOMC), Toulouse, France, 3-7 July, 2011 (http://www.eucomc2011.org/)

J. DRAHOŠ: Honorary committee, 38th International Conference of the Slovak Society of Chemical Engineering (SSCHE), Tatranské Matliare, Slovak Republic, 23-27 May, 2011 (http://sschi.chtf.stuba.sk/konf2011/data/basic_info.html)

J. HANIKA: Programme committee, 45th International Petroleum Conference, Bratislava, Slovak Republic, 13-14 June, 2011 (http://www.vurup.sk/sites/vurup.sk/archivedsite/www.vurup.sk/ipc/index.html)

M. RŮŽIČKA: Program committee, 38th International Conference of the Slovak Society of Chemical Engineering (SSCHE), Tatranské Matliare, Slovak Republic, 23-27 May, 2011 (http://sschi.chtf.stuba.sk/konf2011/data/basic_info.html)

I. WICHTERLE: International Scientific Committee, 25th European Symposium on Applied Thermo-dynamics (ESAT 2011), Saint Petersburg, Russia, 24-27 June, 2011 (http://onlinereg.ru/site.php?go=145&page=2401&lang=ENG)

13TH E. HÁLA LECTURE (2011)

LUDVÍK HUB (Safety Consulting Institute, Binningen, Switzerland)
"Reliability of Methods for the Safety Assessment of Chemical Processes"

ACRONYMS USED THROUGHOUT THE REPORT

ASCR	Academy of Sciences of the Czech Republic
BAS	Bulgarian Academy of Sciences
BINAP	2,2'-bis(diphenylphosphino)-1,1'-binaphthyl
CTU	Czech Technical University in Prague
CU	Charles University in Prague
EFCE	European Federation of Chemical Engineering
EU	European Union
GACR	Grant Agency of the Czech Republic
GA ASCR	Grant Agency of Academy of Sciences 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
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
NMR	Nuclear Magnetic Resonance
PM	Particulate Matter
POPs	Persistent Organic Pollutants
R&D	Research and Development
SAS	Slovak Academy of Sciences
TACR	Technology Agency of the Czech Republic
TU	Technical University
UJEP	Jan Evangelista Purkyně University in Ústí nad Labem
UPa	University of Pardubice
VAST	Vietnam Academy of Science and Technology
VOCs	Volatile Organic Compounds

Annual Report 2011

Vladimír Církva (Editor)

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

Published 2012
Institute of Chemical Process Fundamentals of the ASCR, v. v. i.
Rozvojová 135
165 02 Prague
Czech Republic
www.icpf.cas.cz

Printed 2012
WOW spol. s r.o.
Washingtonova 25
110 00 Prague
Czech Republic
www.wow.cz

ISBN 978-80-86186-37-5