Academy of Sciences of the Czech Republic

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

Praha

ANNUAL REPORT 2009

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ISBN 978-80-86186-22-1

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 center 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 (Research)	Jiří Smolík
Deputy Director (Business Administration)	Olga Šolcová
Scientific Secretary	Jan Linek
Chairman of the Institute Board	Karel Aim

DEPARTMENTS

STAFF

(31 December 2009)

Category	Number of Employees
Research	152
Technical	21
Administrative	14
Services	13

BUDGET 2009

(19 Kč ≈ 1 US$, 26 Kč ≈ 1 EUR)

Resources	Million Kč
Institutional support based on Institutional Research Plan	132
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	51
Foreign R&D Funds and European Programmes	6
Contracts with industry	3
Total Resources	192

Expenses	Per cent of Total Resources
Personal expenses including mandatory insurance	48
Purchase of material	7
Purchase of services	9
Repairs and maintenance	10
Depreciation of fixed assets	17
Travel expenses	3
Energy, water, and fuels	1
Total other expenses	5

Abbreviations used throughout the Report

ASCR	Academy of Sciences of the Czech Republic
CTU	Czech Technical University, Prague
CU	Charles University, Prague
GA CR	Grant Agency of the Czech Republic
ICPF	Institute of Chemical Process Fundamentals of the ASCR, v. v. i., Prague
ICT	Institute of Chemical Technology, Prague
IIC	Institute of Inorganic Chemistry of the ASCR, v. v. i., Prague
IMC	Institute of Macromolecular Chemistry of the ASCR, v. v. i., Prague
IOCB	Institute of Organic Chemistry and Biochemistry of the ASCR, v. v. i., Prague
JH IPC	J. Heyrovský Institute of Physical Chemistry of the ASCR, v. v. i., Prague
MEYS	Ministry of Education, Youth and Sport of the Czech Republic
MIT	Ministry of Industry and Trade of the Czech Republic
TU	Technical University
UJEP	Jan Evangelista Purkyně University, Ústí n/L.
UPa	University of Pardubice

Department of Separation Processes

Head:	V. Jiřičný
Deputy:	J. Křišťál
Research staff:	J. Hanika, A. Heyberger, P. Izák, M. Kohoutová, R. Petričkovič, K. Rochová, M. Rousková, J. Řezníčková, M. Sajfrtová, K. Setničková, P. Stavárek, P. Uchytil Part time: H. Sovová, V. Staněk, Z. Vajglová, M. Veselý, E. Volaufová, H. Vychodilová
Technical staff:	A. Kadlecová, D. Karfík, M. Koptová, J. Maščeník, D. Vlček
PhD students:	V. Jarmarová, M. Poloncarzová, B. Vokatá, P. Záloha

Fields of research

- Research and development of electrochemical bipolar microreactor for electrochemical alkoxylation process
- Hydrodynamics of two phase flow in narrow channel
- Sulfur dioxide oxidation, sulfation and sulfonation
- Liquid-liquid extraction of tall oil from wastewaters of paper industry
- Fluorinated hydrocarbons as potential solvents in liquid-liquid extraction processes
- Extraction of luminophores
- Supercritical fluid extraction of biologically active substances
- Enzymatic reactions in supercritical CO_2
- Study of mass transport during vapour permeation and pervaporation in polymeric membranes
- Study of vapour condensation effect in ceramic membranes pores
- Separation of racemic mixtures
- Separation of gasoline vapours from air by supported ionic liquids membranes
- Purification of biogas by supported ionic liquid membrane

Applied research

- Research and development of new methods of emulsification using microtechnology
- Extraction of polyaromatic hydrocarbons from aromatic petroleum fraction (300–400 ^{o}C)
- Extraction and production of plastic modifiers for production of tyres
- Liquid extraction of luminophores, recycling of Y and Eu
- Extraction and refining of plant extracts

Research projects

Integrated multiscale process units with locally structured elements (IMPULSE)
(J. Hanika, V. Jiřičný, J. Drahoš, 6th FP integrated project, Priority 3 NMP, supported by EU under Contract No. 011816-2)

The objective of IMPULSE project is effective, targeted integration of innovative process equipment such as microreactors, heat exchangers, thin-film devices and other micro components to attain radical performance enhancement for whole process systems in chemical production. We are involved in the application research of electroorganic synthesis in electrochemical microreactor. Bipolar electrochemical microreactors proved advantageous of microtechnology. While conversion and selectivity of the process are comparable with conventional process, the main profit of applied microtechnology is in less expensive separation of the product from reaction mixture. [Refs. 9, 10, 18, 21, 36, 63, 64]

Flexible, fast and future production processes (F3 Factory)
(V. Jiřičný, 7th FP collaborative large integrated project, Theme NMP-2008-3.2-1, supported by EU under Contract No CP-IP 228867-2 F3 Factory)

The goals of the projects are in improvements of EU chemical industry's competitive position by development modular continuous plant (F3 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. Project started in June 2009. We are involved in research and developments of sulfur dioxide oxidation, sulfation and sulfonation.

Chemical degradation of polybrominated diphenyl ethers
(V. Jiřičný, supported by GA CR, project No. GA104/09/0880)

Polybrominated diphenyl ethers (PBDE) are widely used as flame retardants, mainly for polymers and textiles. PBDE have an ideal property for these matrices because they are decomposed at temperature 50 °C lower than point of flammability of matrix. PBDE are pollutants of environment. They are lipophilic, potential carcinogenic and neurotoxic compounds, which accumulate in environment and they can migrate by food chain into human organisms. The project (opened in 2009) deals with various methods of degradation of polybrominated diphenyl ethers. During first year the analytical methods have been developed and first experiments with reductive degradation of PBDE utilizing bimetallic Pd/Fe catalysts and in photochemical reactor by TiO_2 catalyst were conducted.

Research and developments of new methods of emulsification using microtechnology
(J. Křišťál, contract with Procter&Gamble, ICPF Contract No. 1719)

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 P&G research reports.

Reclaiming of phytosterols and other valuable compounds from tall soap/oil
(A. Heyberger, joint project with Technological Park Chomutov and Institute of Systems Biology and Ecology of the ASCR, v. v. i., supported by ASCR, project No. 1QS400720504)

The aim of the project is to study the tall soap composition and to develop methods of extractive separation of the valuable compounds. Besides of working out the necessary analytical methods, the extraction equilibria in systems with various solvents are measured,

and the separation processes will be simulated in a laboratory vibrating plate extraction column. A novel extraction processes and equipment will be designed for recovering phytosterols and unsaturated fatty acids from tall soap. [Refs. 26, 34, 47, 48]

Supramolecular materials based on natural phytosterols for applications in biology
(H. Sovová, joint project with IOCB, ICT, and Chemispol, supported by MEYS, project No. 2B06024)

The effect of extraction conditions for the content of beta-sitosterol in CO_2 extracts from seeds was described [Ref. 52] and a method for quantification of free and conjugated sterols in plants was improved [Ref. 40]. The influence of flow direction in supercritical fluid extractor on its performance was investigated [Ref. 45]. The potential of enzymatic reactions of vegetable oils in supercritical carbon dioxide to enhance the concentration of sterols was examined [Refs. 6, 11, 46, 53, 54].

Optimization of supercritical fluid extraction for maximal yield of biologically active substances from plants
(H. Sovová, joint project with Research Institute of Plant Production and Agra Group, supported by MEYS, project No. 2B06049)

Extracts from savory and thymus were obtained by different separation methods. The composition of volatile compounds in the extracts was determined and the toxicity and antifeedant effects of the extracts on larvae of Colorado potato beetle were evaluated. The lowest lethal dosages were 0.022 mg for essential oil and 0.028 mg for supercritical extract of savory. Strong deterrent effects of all extracts against larvae were observed [Ref. 12]. Different mathematical models for the rate of supercritical fluid extraction were critically reviewed [Ref. 22]. The data on insecticidal activity of the isolates from several other aromatic plants were published [Refs. 50, 51].

Determination of biological activity and chemical composition of selected tropical and subtropical Ranunculaceae species
(H. Sovová, joint project with Czech University of Life Sciences, and IOCB, supported by GACR, grant No. GA525/08/1179)

The research was focused on the enhancement of thymoquinone concentration in CO_2 extracts of black cumin (*Nigella sativa* L.) seeds. The composition of volatile oil in the extracts was strongly influenced by extraction pressure (12 – 28 MPa). Mild extraction conditions (12 MPa and 50 °C) allowed us to separate the volatile oil from fatty oil and, using the solvent-to-feed ratio 3.7 g/g, reach a high concentration of thymoquinone in the extract, 20 mass %. [Ref. 49]

Study of polymeric membrane swelling and make use of this effect for increasing its permeability
(P. Uchytil, joint project with IMC, supported by the GACR, Grant No. GA104/09/1165)

Transport of carbon dioxide and methane through dense homogeneous polyethersulfone membranes filled with different contents (0, 10, and 20 mass %) of sodium montmorillonite (Na-MMT, basal spacing ≈ 1.39 nm) was studied. Gas permeation measurements were conducted using a semi-open cell which is divided into two parts by the membrane. A constant pressure was maintained at the feed side, while a vacuum was created at the permeate side in the beginning of experiment. The increase of permeate pressure with the time was recorded, and from this dependence, the gas flux and the permeability were evaluated [Ref. 62]. The flow of saturated vapors through porous Vycor glass was investigated theoretically and experimentally [Refs. 39, 58].

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

(P. Uchytil, joint project with National Chung Hsing University, Taiwan, supported by ASCR and by National Science Council of Taiwan)

The project is focused on the membrane preparation or their modification as well as the application in gas-phase separation processes. Some membranes on the basis of polyethersulfone and cellulose acetate filled with zeolite nanoparticles were prepared and their transport parameters and separation ability were tested by dynamic permeation method.

Mass transport during membrane permeation and pervaporation

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

A new method for the evaluation of the gas separation ability of ionic liquids was proposed. A key point is the preparation of an unbroken ionic liquid layer between two polymer layers. The thin layer of an ionic liquid was deposited on the surface of a polymeric material. Then the free surface of ionic liquid was covered by another sample of the same polymeric material and the so called "sandwich sample", in which the ionic liquid is closed between two layers of a polymer, was prepared for gas permeation experiments. Transport properties of the ionic liquid (1-hexyl-3-methylimidazolium) were tested by the measurements of carbon dioxide and methane permeation. The polymeric material is a dense polyethersulfone (PES) membrane filled with 20 wt % of sodium montmorillonite (thickness 25 μm). The thickness of the ionic liquid layer between the two polymeric membranes was calculated from its weight and it was estimated to be 13 μm. The obtained results had shown that the ionic liquid (1-hexyl-3-methylimidazolium) exhibits good separation properties for system CO_2/CH_4 (ideal separation factor $\alpha = 60$) with carbon dioxide permeability 1.5×10^{-15} mol.m.m^{-2}.s^{-1}.Pa^{-1}. Ref. 59]

Ionic membranes for selective separation of liquid mixtures by pervaporation

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

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 ionic liquids 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. [Refs. 7, 8]

Purification of biogas by supported ionic liquid membrane

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

The goal of this work is to find a way to lower concentration of carbon dioxide in biogas, to remove undesirable gases and to increase methane concentration up to 95 % by means of membranes. Sweeping gas permeation is performed with model mixture of CO_2, CH_4 and H_2S.

International co-operations

CNRS Toulouse, France: Characterization of two phase flow in microchannels
Procter&Gamble, Belgium: Research and development of new methods of emulsification using microtechnology
CNRS Lyon: Hydrogenation in falling film microreactor
Slovak University of Technology in Bratislava, Slovakia: Processing of tall soap/oil extraction products
CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials
University of KwaZulu-Natal, Republic of South Africa: Liquid-liquid extraction processes
Institute of Chemical Engineering, Sofia, Bulgarian AS: High-pressure phase equilibria
Institute of Macromolecules, St. Petersburg, Russian Academy of Science, Russia: Membrane separation
Otto von Guericke University of Magdeburg, Magdeburg, Germany: Mass transport through porous membranes
Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapors through porous membranes
University of Linz, Linz, Austria: Determination of organic pollutants in water
Technical University of Lisbon, Portugal: Supercritical extraction of biological compounds from aromatic plants
University of Colorado, Boulder, USA: Mass transport during vapour permeation and pervaporation, ionic liquids
National Chung Hsing University, Taiwan: Preparation of Dense Homogeneous Polymeric Membranes and Study on Their Gas Permeation Properties

Visits abroad

A. Heyberger: CSIR of Johannesburg, University of KwaZulu-Natal, Durban, South Africa (1 month)
J. Křišťál: Procter & Gamble, Brussels, Belgium (3 months)
P. Stavárek: CNRS Lyon, France (8 months)

Visitors

J. Aubin, CNRS Toulouse, France
M. Botha, University of KwaZulu-Natal, Durban, Republic of South Africa
M. Čársky, University of KwaZulu-Natal, Durban, Republic of South Africa
P. Dufour, Université Claude Bernard, Lyon, France
A. Palavra, Technical University of Lisbon, Portugal
H. Melin, ENSIASET, Toulouse, France

Teaching

J. Hanika: ICT, course and postgradual course "Multiphase reactors"
J. Hanika: ICT, course "Pharmaceutical engineering"
J. Hanika: UPa, course "Industrial catalysis"
H. Sovová: ICT, postgraduate course "Properties and application of supercritical fluids"

Publications

Original papers

1. Dudas J., Hanika J.: Design, Scale up and Safe Piloting of Thymol Hydrogenation and Menthol Racemisation. Chem. Eng. Res. Des. 87(1), 83-90 (2009).
2. Friess K., Jansen J.C., Vopička O., Randová A., Hynek V., Šípek M., Bartovská L., Izák P., Dingemans M., Dewulf J., Van Langenhove H., Drioli E.: Comparative Study of Sorption and Permeation Techniques for the Determination of Heptane and Toluene Transport in Polyethylene Membranes. J. Membr. Sci. 338(1-2), 161-174 (2009).
3. Gogová Z., Hanika J.: Reactivation of a Palladium Catalyst during Glucose Oxidation by Molecular Oxygen. Chem. Pap. 63(5), 520-526 (2009).
4. Gogová Z., Hanika J.: Dynamic Modelling of Glucose Oxidation with Palladium Catalyst Deactivation in Multifunctional CSTR; Benefits of Periodic Operation. Chem. Eng. J. 150(1), 223-230 (2009).
5. Gogová Z., Hanika J.: Model-Aided Design of Three-Phase Gas-Lift Reactor for Oxidation Accompanied by Catalyst Reversible Deactivation. Chem. Eng. Technol. 32(12), 1929-1940 (2009).
6. Hlavsová K., Zarevúcka M., Wimmer Z., Macková M., Sovová H.: Geotrichum candidum 4013: Extracellular Lipase versus Cell-bound Lipase from the Single Strain. J. Mol. Catal. B - Enzym 61(3-4), 188-193 (2009).
7. Izák P., Friess K., Hynek V., Ruth W., Fei Z., Dyson J.P., Kragl U.: Separation Properties of Supported Ionic Liquid-Polydimethylsiloxane Membrane in Pervaporation Process. Desalination 241(1-3), 182-187 (2009).
8. Kohoutová M., Sikora A., Hovorka Š., Randová A., Schauer J., Tišma J., Setničková K., Petričkovič R., Guernik S., Greenspoon N., Izák P.: Influence of Ionic Liquid Content on Properties of Dense Polymer Membranes. Eur. Polym. J. 45(3), 813-819 (2009).
9. Křišťál J., Jiřičný V.: Integrovaný EU projekt IMPULSE přinesl zajímavé výsledky. (Czech) Integrated EU Project IMPULSE Delivered Interested Results. CHEMagazín 19(4), 18-19 (2009).
10. Křišťál J., Jiřičný V.: Integrovaný EU projekt IMPULSE přinesl zajímavé výsledky. (Czech) Integrated EU Project IMPULSE Delivered Interested Results. Chem. Listy 103(4), 352-354 (2009).
11. Lísa M., Holčapek M., Sovová H.: Comparison of Various Types of Stationary Phases in Non-Aqueous Reversed-Phase High-Performance Liquid Chromatography–Mass Spectrometry of Glycerolipids in Blackcurrant Oil and its Enzymatic Hydrolysis Mixture. J. Chromatogr. A 1216(47), 8371–8378 (2009).
12. Pavela R., Sajfrtová M., Sovová H., Karban J., Bárnet M.: The Effects of Extracts Obtained by Supercritical Fluid Extraction and Traditional Extraction Techniques on Larvae Leptinotarsa decemlineata SAY. J. Essent. Oil Res. 21(4), 1-7 (2009).
13. Randová A., Bartovská L., Hovorka Š., Poloncarzová M., Kolská Z., Izák P.: Application of the Group Contribution Approach to Nafion Swelling. J. Appl. Polym. Sci. 111(4), 1745-1750 (2009).
14. Smejkal Q., Kolena J., Hanika J.: Ethyl Acetate Synthesis by Coupling of Fixed-bed Reactor and Reactive Distillation Column—Process Integration Aspects. Chem. Eng. J. 154(1-3), 236-240 (2009).
15. Staněk V., Hanika J., Jiřičný V., Stavárek P., Tukač V., Lederer J: Prediction of Improved Performance of Catalytic Hydrogenation Reactor by Periodic Modulation of the Feed Rate. Chem. Industry Chem. Eng. Q. 23(3), 251-257 (2009).
16. Tukač V., Hanika J., Veselý V., Lederer J., Nečesaný F.: Možnosti produkce vodíku parciální oxidací odpadní biomasy. (Czech) Possibility of Hydrogen Production by Partial Oxidation of Waste Biomass. CHEMagazín 19(3), 8-9 (2009).
17. Veselý V., Hanika J., Drahoš J.: Petelýza, chemická recyklace PET lahví. (Czech) Petelysis, Chemical Recycling of PET Bottles. Waste Forum 26-29 (2009).

18. Bouzek K., Jiřičný V., Kodým R., Křišťál J., Bystroň T.: Microstructured Reactors for Electroorganic Synthesis. Electrochim. Acta, in press.
19. Petričkovič R., Setničková K., Uchytil P.: New Apparatus for Gas Permeability, Diffusivity and Solubility Assessing in Dense Polymeric Membranes. J. Membr. Sci., submitted.
20. Procházka J., Heyberger A., Volaufová E.: Effect of Diluents on Sulfuric Acid Extraction with Trialkylamine. AIChE J., submitted.

Review papers

21. Aubin J., Ferrando M., Jiřičný V.: Current Methods for Characterising Mixing and Flow in Microchannels: A Review. Chem. Eng. Sci., in press.

Chapters in books

22. Sovová H.: Mathematical Modelling of Supercritical Fluid Extraction. In: Current Trends of the Supercritical Fluid Technology in the Pharmaceutical, Nutraceutical and Food Processing Industries. (Duarte, A.R.C., Duarte, C. M. M., Ed.), pp. 1-15, Bentham eBooks 2009.
23. Evans J.W., Jiřičný V.: Chapter 16: Spouted Bed Electrolytic Reactors. In: Spouted and Spout Fluid Beds: Fundamentals and Applications. (Epstein, N., Ed.), Cambridge Press, London, in press.
24. Izák P., Friess K., Šípek M.: Permeation and Pervaporation Taking Advantage of Ionic Liquids. In: Membranes: Properties, Performance and Applications. (Columbus, F., Ed.), Nova Science Publishers, in press.

Patents

25. Novák L., Černín A., Hanika J., Veselý V.: Způsob a zařízení pro izolaci kyseliny tereftalové. (Czech) Princip and Device for Terephthalic Acid Isolation. Pat. No. PV 2008-602/CZ 301168. Applied: 08.10.09, Patented: 09.10.15.
26. Heyberger A., Tříska J., Rousková M., Krtička M.: Způsob a zařízení k získávání fytosterolů. (Czech) Process and Equipment for Phytosterols Recovering. Pat. No. PV 2008-852. Applied: 08.12.30.

International conferences

27. Bouzek K., Fíla V., Jiřičný V.: Strukturované aparáty. Nový přístup k návrhu chemických technologií. (Czech) Structured Apparatuses – New Way in Design of Chemical Technologies. 18. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, orally, Milovy, Czech Republic, 20-22 April 2009.
28. Bradová M., Hanika J., Veselý V.: Čištění tereftalátu membránovou technologií. (Czech) Terephthalate Purification by Membrane Technology. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 104, Srní, Šumava, Czech Republic, 19-22 October 2009.
29. Fialová K., Petričkovič M., Uchytil P.: New Apparatus for Permeation Experiments. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, Tatranské Matliare, Slovakia, 25-29 May 2009.
30. Gogová Z., Hanika J.: Composition Modulation of Catalytic Reactors. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 84 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
31. Gogová Z., Hanika J.: Multifunctional Reactors for Oxidation Accompanied with Reversible Catalyst Deactivation. 8th World Congress of Chemical Engineering (WCCE8), Abstract Book, p. 1172 (6 pp. full text on CD-ROM), Montreal, Canada, 23-27 August 2009.
32. Hanika J., Lederer J., Nečesaný F., Tukač V., Veselý V.: Produkce vodíku současnou parciální oxidací odpadní biomasy a ropných zbytků. (Czech) Hydrogen Production by Partial Oxidation of Biomass and Crude Oil Wastes. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 48 (10 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
33. Hanika J., Lederer J., Nečesaný F., Tukač V., Veselý V.: Možnosti produkce vodíku parciální oxidací odpadní biomasy. (Czech) Possibility of Hydrogen Production by Partial Oxidation of Waste Biomass. Seminář Biopaliva v dopravě, Book of Abstracts, 8 pp. full text on CD-ROM, Bratislava, Slovakia, 21-22 September 2009.

34. Heyberger A., Rousková M., Čársky M.: Liquid-Liquid Extraction of Phytosterols from Tall Soap. South African Chemical Engineering Congress 2009, Book of Abstracts and Programme, p.26 (9 pp. full text on CD-ROM)), Somerset West, South Africa, 20-23 September 2009.
35. Izák P., Kohoutová M., Afonso C.A.M., Crespo J. G.: Využití pervaporace pro zvýšení efektivnosti reakčního procesu. (Czech) Pervaporation as a Tool for Higher Effectiveness of Reaction Process. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 42 (8 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
36. Jiřičný V., Vychodilová H., Melich Z., Kodým R., Bystroň T., Bouzek K.: Vývoj bipolárního elektrochemického mikroreaktoru pro organické syntézy. (Czech) Development of Bipolar Electrochemical Microreactor for Organic Synthesis. 18. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2009, Sborník přednášek, pp. 2211-2218, Milovy, Czech Republic, 20-22 April 2009.
37. Kohoutová M., Sikora A., Hovorka Š., Randová A., Schauer J., Setničková K., Petričkovič R., Poloncarzová M., Izák P.: How Ionic Liquids Change Properties of Polymeric Membranes. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 284, Tatranské Matliare, Slovakia, 25-29 May 2009.
38. Kohoutová M., Sikora A., Hovorka Š., Randová A., Schauer J., Izák P.: Influence of Ionic Liquid Content on Properties of Dense Polymer Membranes. PERMEA 2009, Programme Booklet, p. 87, Prague, Czech Republic, 07-11 June 2009.
39. Loimer T., Uchytil P., Petričkovič R., Setničková K.: The Flow of Saturated Vapors through Porous Vycor Glass. 4th International Conference on Applications of Porous Media, Proceedings Book, pp. 126-131, Istanbul, Turkey, 10-12 August 2009.
40. Pavlík M., Siglerová V., Wimmer Z., Sovová H., Sajfrtová M., Pavlíková D.: Micro-Extraction of Hydrolyzed Free and Conjugated Sterols for Their Determination Using HPLC. 34th FEBS Congress, Volume 276 Issue s1, pp. 288-289, Prague, Czech Republic, 04-09 July 2009.
41. Poloncarzová M., Bartovská L., Randová A., Hovorka Š., Izák P.: Určení kritické micelární koncentrace pomocí měření kontaktního úhlu. (Czech) Determination of Critical Micelle Concentration from Contact Angle Measurement. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 244, Srní, Šumava, Czech Republic, 19-22 October 2009.
42. Poloncarzová M., Kohoutová M., Izák P.: Separace organických par ze vzduchu pomocí zakotvených iontových membrán. (Czech) Separation of Volatile Organic Compounds from Air by Supported Ionic Liquid Membranes. 18. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, Milovy, Czech Republic, 20-22 April 2009.
43. Randová A., Bartovská L., Hovorka Š., Izák P., Friess K.: Sorption Behaviour of Polyethylene + Toluene + Lower C1 – C6 Aliphatic Alcohols Systems. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 246, Tatranské Matliare, Slovakia, 25-29 May 2009.
44. Randová A., Bartovská L., Hovorka Š., Izák P., Friess K.: Low Density Polyethylene in Organic Liquids. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 224, Tatranské Matliare, Slovakia, 25-29 May 2009.
45. Rochová K., Sovová H.: Effect of Flow Direction on Axial Dispersion in Supercritical Extractor. 9th International Symposium on Supercritical Fluids, Abstracts, p. 287 (P139), Arcachon, France, 18-20 May 2009.
46. Rochová K., Sovová H., Zarevúcka M.: Enzymatické reakce v superkritickém CO_2. (Czech) Enzymatic Reactions in Supercritical CO_2. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 86 (6 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
47. Rousková M., Heyberger A., Tříska J.: Získávání fytosterolů z tálového mýdla kapalinovou extrakcí. (Czech) Recovery of Phytosterols from Tall Soap Using Liquid-Liquid Extraction. 18. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, pp. 1217-1222, Milovy, Czech Republic, 20-22 April 2009.
48. Rousková M., Heyberger A., Volaufová E., Tříska J., Krtička M.: The Effect of Tall Soap pH Adjustment on Extract Composition. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 197 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
49. Sajfrtová M., Karban J., Klouček P., Malík J., Kokoška L: Supercritical Fluid Fractionation for Thymoquinone Enrichment in Black Cumin and Savory Isolates. 57th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research, Abstracts, Planta Medica 9(75), 1041, 2009, Geneva, Switzerland, 16-20 August 2009.
50. Sajfrtová M., Rochová K., Karban J., Sovová H., Pavela R.: Insecticide Activity of Peppermint and Lavender Extracts Isolated by Different Methods. 57th International Congress and Annual Meeting of the

Society for Medicinal Plant and Natural Product Research, Abstracts, Planta Medica 9(75), 1053, 2009, Geneva, Switzerland, 16-20 August 2009.

51. Sajfrtová M., Sovová H., Karban J., Pavela R.: Využití superkritické extrakce pro izolaci botanických insekticidů. (Czech) Utilization of Supercritical Fluid Extraction for Botanical Insecticide Isolation. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 143, Srní, Šumava, Czech Republic, 19-22 October 2009.
52. Rochová K., Sovová H., Sajfrtová M., Bártlová M., Wimmer Z.: Preparation of Extracts Rich in beta-Sitosterol Using Supercritical CO_2. 2nd International Congress on Green Process Engineering, Proceedings, Venice, Italy, 14-17 June 2009.
53. Sajfrtová M., Zarevúcka M., Sovová H., Rochová K.: Enzyme-catalyzed Reaction of Vegetable Oil in Supercritical CO_2 in a Continuous-flow Reactor. 2nd International Congress on Green Process Engineering, Proceedings, Venice, Italy, 14-17 June 2009.
54. Sajfrtová M., Zarevúcka M., Sovová H.: Enzyme-catalyzed Reaction of Vegetable Oil in Supercritical CO_2 in a Continuous-flow Reactor. 9th International Symposium on Supercritical Fluids, Abstracts, p. 204 (P056), Arcachon, France, 18-20 May 2009.
55. Setničková K., Jeřábek K., Uchytil P.: Pervaporace versus permeace par – rozdíly z hlediska transportu látek polymerní membránou. (Czech) Pervaporation vs. Vapor Permeation - Differences in Transport Properties of the Polymeric Membrane. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 44, Srní, Šumava, Czech Republic, 19-22 October 2009.
56. Tukač V., Handlová M., Sazanov Z., Lederer J., Kolena J., Kubička D., Hanika J., Jiřičný V.: Intenzifikace pilotního zkrápěného reaktoru periodickou modulací nástřiku. (Czech) Intensification of Pilot Plant Trickle Bed Reactor by Feed Rate Periodic Modulation. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 28 (8 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
57. Tukač V., Tomešová Z., Hanika J., Veselý V., Lederer J., Nečesaný F.: Možnosti produkce vodíku parciální oxidací odpadní biomasy. (Czech) Potential Hydrogen Production by Partial Oxidation of Waste Biomass. 18. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, pp. 1140-1147, Milovy, Czech Republic, 20-22 April 2009.
58. Uchytil P.: Transport of Condensable Gas (Butane) in Vycor Membrane. 2nd International Symposium on Inorganic Membranes, Invited lecture, Higashi-Hiroshima, Japan, 15 July 2009.
59. Uchytil P., Noble R., Wu J.-W., Petričkovič R., Suen S.-Y.: Testing of Ionic Liquid Transport Properties. 19th Annual Meeting of the North American Membrane Society, Programe, Poster 13, Charleston, South Carolina, USA, 20-24 June 2009.
60. Veselý V., Hanika J.: Ekonomika chemické recyklace PET lahví. (Czech) Economics of PET Bottles Chemical Recycling. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 51, Srní, Šumava, Czech Republic, 19-22 October 2009.
61. Vopička O., Hynek V., Zgažar M., Friess K., Izák P.: Sorption and Permeation Properties of Ionic Liquid-Silicone Blends for Butanol Vapours. PERMEA 2009, Programme Booklet, p. 173, Prague, Czech Republic, 07-11 June 2009.
62. Wu J.-W., Suen S.-Y., Petričkovič R., Uchytil P.: Na-montmorillonite-filled Polyethersulfone Membranes for Gas Transport. 5th Conference of Aseanian Membrane Society, Book and Abstracts, p. 183(P5-50), Kobe, Japan, 12-14 July 2009.
63. Záloha P., Křišťál J., Jiřičný V.: Vizualizace dvoufázového toku v elektrochemickém mikroreaktoru. (Czech) Visualization of Two-Phase Flow in Electrochemical Microreactor. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 111 (10 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
64. Stavárek P., Le Doan T.V., Loeb P., de Bellefon C.: Flow Visualization and Mass Transfer Characterization of Falling Film Reactor. 8th World Congress of Chemical Engineering, Abstract Book, p. 213, Montreal, Canada, 23-27 August 2009.

E. Hála Laboratory of Thermodynamics

Head: K. Aim
Deputy: M. Lísal
Research staff: M. Bendová, J. Jirsák, J. Linek, L. Morávková, J. Pavlíček, Z. Sedláková, L. Vlček, Z. Wagner, I. Wichterle
Part time: A. Malijevský, M. Malý, I. Nezbeda, P. Petrus, Z. Posel, M. Předota
Technical staff: S. Bernatová
PhD student: K. Machanová

Fields of research

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

Applied research

- Novel technology for preparation of molecularly imprinted polymeric materials

Research projects

Determination of the phase and state behaviour of fluids and fluid mixtures for processes at superambient conditions: molecular-based theory and experiment
(K. Aim, joint project with UJEP and CTU, supported by ASCR, grant No. IAA400720710)

Research was focused on interpretation of results obtained in the framework of perturbation methods. It was shown that the inclusion of a short-range part of the total

attractive interaction into a reference system allows a natural extension of the traditional first-order perturbation theory of simple fluids to practically all thermodynamic states. Research continued on applications of the perturbation theory using a reference system based on the short-range part of intermolecular interactions to describe the thermodynamic behaviour of systems containing carbon dioxide + alkanols. The measurements of liquid-liquid equilibria in binary systems of 1-ethyl-3-methylimidazolium ethyl sulphate + n-heptane / + methylcyclo-hexane / + toluene were completed and the data obtained were successfully represented by polymer-solution models. [Refs. 2, 7, 12, 24, 25, 27, 42]

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

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

Densities and sound velocities were measured for binary systems composed of isooctane, toluene, and MTBE at four temperatures within 298.15 K and 328.15 K and atmospheric pressure. Statistic and gnostic methods were applied to fit the incomplete data of excess volumes [Refs. 8, 32]. Volumetric properties of pyridine, 2-picoline, 3-picoline, and 4-picoline at temperatures from 298.15 K to 328.15 K and at pressures up to 40 MPa were determined experimentally [Ref. 18]. In addition to it, volumetric behaviour of ternary liquid system composed of toluene, isooctane, and methyl tert-butyl ether at temperatures from 298.15 K to 328.15 K was measured and correlated to determine the necessary number of ternary constants to fit the experimental data within the experimental error [Refs. 30, 31].

Molecular simulations at extreme experimental conditions: Application of advanced methods to geochemistry

(M. Lísal, supported by ASCR, project No. 1ET400720507)

New methods and algorithms for computer modelling and molecular simulations in geochemistry (particularly for geological fluid systems at extreme state conditions) have been developed. The main pursued lines of research were (i) state and phase behaviour of geological fluids at high temperatures and high pressures and (ii) physico-chemical properties of geological fluid systems in porous media. To this end, molecular simulation methodologies and density functional theory for non-reacting and high-density chemically-reacting fluid systems both in the bulk and in confinement have been developed and tested. [Refs. 5, 11, 37, 42]

Design of "tailor made" multifunctional organic materials by molecular modelling of structure – property relationship, experimentation and processing (MULTIPRO)

(M. Lísal, supported by FP6 RTD EU, project No. NMP3-CT-2006-033304)

The aim of MULTIPRO is to develop new multifunctional materials for opto-electronic devices based on solid state lighting sources, addressed to several applications (automotive head-up displays and lighting, public information displays and general lighting) and, at the same time, a new integrated reactive packaging technology suitable for the material developed and cost effective for the applications. MULTIPRO develops polymeric resins in which nanoparticles of different nature are built in or embedded in order to reach multifunctional material with new and improved properties. The specific material properties are controlled and tailored by changing nature, size, composition, and concentration of the nanoparticles according to industrial and technological request. MULTIPRO responds to the concept of the "tailor made", which means that the above described functionalities respond to specific needs of a given application. Molecular modelling is the enabling technology to tailor the material in terms of components necessary for the properties desired. MULTIPRO also develops modelling procedures and dedicated software to simulate each step of materials

development from the pure components structure to reactive models, up to the final materials, from which properties can be argued. [Refs. 4, 11]

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

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

The aim of the project is to study the behavior of fluids in the nanospace, solid-liquid interface (metal oxide-aqueous solution) and nanoporous carbons (activated carbons and carbon nanotubes) by equilibrium and nonequilibrium molecular simulations to provide structural, dynamical and transport properties of fluids in nanoconfinement. At solid-liquid interfaces, the simulation results for dynamics of water molecules are linked with quasielastic neutron scattering; the space-dependent shear viscosity and the dielectric properties are linked with electrophoretic data. We are also developing a method for the determination of local, space-dependent permittivity in inhomogeneous systems. In the case of nanoporous carbons, we adopt the methods for calculating local, space-dependent diffusivity and shear viscosity of pure fluids to slit and cylindrical nanopores, develop a method for the determination of space-dependent shear viscosity of fluid mixtures from computer simulations, and simulate the structural, dynamical and transport properties of industrially important fluid mixtures in carbon nanopores. [Refs. 6, 35, 36, 38]

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

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

A brand new Monte Carlo simulation method, MPM-MC (multi-particle move MC) developed in 2008, has been implemented for two different Hamiltonians and then applied to the water-methanol mixture with polarizable interactions. To our best knowledge, this was the first simulation result which yielded the minimum in the partial molar volume of methanol. Since water is in the focus of the entire project, two studies [Refs. 12, 13] dealt with non-additive interactions. [Refs. 9, 10, 12, 13, 33, 34, 41, 43]

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

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

A new apparatus for measurements of high-pressure phase equilibria by synthetic method was assembled, based on Thar Technologies Super Phase Monitor. The accuracy of the apparatus was first checked by measuring the solubilities of supercritical CO_2 in ethanol or butanol. Subsequently, solubilities of supercritical CO_2 in ionic liquid 1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide were measured. Due to the easy recyclability of ionic liquids, binary systems of amines and ionic liquids are investigated for potential carbon dioxide capture use; related solid-liquid equilibria in system diethylamine + [emim][NTf_2] have been studied. Experimental SLE data were correlated by using the Redlich-Kister equation and compared with calculated ideal solubilities. [Refs. 39, 40]

Thermodynamic properties of gas-liquid systems

(I. Wichterle, supported by GACR, grant No. GA104/07/0444)

Vapour–liquid equilibria in 9 binary and 3 ternary systems of species with selected functional groups (tert-butyl, isopropyl, carbonyl, ether, and hydroxyl) have been measured. Liquid–liquid equilibrium data were determined in systems ionic liquid + water/alcohol/hydrocarbon. New microebulliometer for total pressure measurement was developed and tested. An algorithm for reliable evaluation of temperature-independent

parameters from vapour–liquid equilibria at high pressures was developed. [Refs. 3, 15, 19, 21, 25, 39, 40]

Novel technology of preparation of molecularly imprinted polymeric materials
(I. Wichterle, supported by Ministry of Science, Education and Sports of Croatia, project No. MZOS-RH 061-0-3029)

Copolymers and terpolymers synthesized by polymerization of long chain methacrylates with styrene and (meth)acrylic acid with styrene or 1-vinyl-2-pyrrolidone are efficient flow improvers for oil transport. Liquid–vapour equilibria for solutions of these polymers in toluene were determined by micro-ebulliometry at different temperatures and pressures. A new computer programme for the modelling of physico–chemical properties of oil was developed. Data on miscibility and phase behavior of binary polymer blends were compiled and published in a book. [Refs. 23, 28, 29]

EFCE Working Party "Fluid Separations"
(M. Bendova, supported by MEYS, programme INGO project No. LA320)

Activities connected with membership of M. Bendova in EFCE Working Party on "Fluid separations". Dr. Bendova took part in the annual WP meeting at the ENSIACET in Toulouse, France, on May 27 – 30, 2009. [Ref. 1]

International co-operations

Technical University of Vienna, Austria: Colloids and theory of fluids
University of Ontario Institute of Technology, Oshawa, ON, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids
INA, Research and Development, Zagreb, Croatia: Properties of polymer solutions
Université François Rabelais, Tours, France: Liquid-liquid phase equilibria in systems of ionic liquids
University of Leipzig, Leipzig, Germany: Fluids at extreme conditions
DICAMP, University of Trieste, Italy: Phase equilibria for supercritical fluid technology
University of Ljubljana, Ljubljana, Slovenia: Water and hydration of nonpolar and ionic solutes
Institute of Condensed Matter, Ukrainian Acad. Sci., Lviv, Ukraine: Modelling of molecular fluids at extreme conditions: Theory and applications
Queen's University Ionic Liquids Laboratory (QUILL), Belfast, UK: Liquid-liquid phase equilibria in systems of ionic liquids
U. S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale simulations of energetic and reactive materials
Pennsylvania State University, State College, PA, USA: Dissipative particle dynamics simulations of adsorption behaviour of model proteins on surface
Oak Ridge National Laboratory, Oak Ridge, TN, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems

Visits abroad

J. Jirsák: University of Ontario, Institute of Technology, Oshawa, ON, Canada (7 months)

M. Lísal: University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)
M. Lísal: Pennsylvania State University, State College, PA, USA (1 month)
A. Malijevský: Imperial College, London, UK (8 months)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

A. Trokhymchuk, Institute of Condensed Matter Physics, Lviv, Ukraine
R. Melnyk, Institute of Condensed Matter Physics, Lviv, Ukraine

Teaching

M. Lísal: UJEP, courses "Parallel programming", "Numerical mathematics I" and "Numerical mathematics II"; tutorials "Molecular simulations I"
I. Nezbeda: UJEP, courses "Molecular simulations I", "Molecular theory of matter", "Kinetic theory", "Principles of Scientific Communication" and "Statistical Physics"
I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"
M. Kotrla, M. Předota: CU, course "Advanced computer simulations in many particle systems"
M. Předota: University of South Bohemia, Č. Budějovice, courses "Lectures from physics oriented to particle and nuclear physics" and "Selected lectures from physics"

Publications

Original papers

1. Bendová M.: Konference Distillation and Absorption 2010. (Czech) Conference Distillation and Absorption 2010. Chem. Listy 103(10), 862 (2009).
2. Bendová M., Wagner Z.: Thermodynamic Description of Liquid-Liquid Equilibria in Systems 1-Ethyl-3-methylimidazolium Ethyl sulfate + C7-Hydrocarbons by Polymer-Solution Models. Fluid Phase Equilib. 284(2), 80-85 (2009).
3. Bernatová S., Pavlíček J., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of tert-Butyl Methyl Ether, 3,3-Dimethyl-2-butanone and 2,2-Dimethyl-1-propanol. Fluid Phase Equilib. 278(1-2), 129-134 (2009).
4. Brennan J.K., Lísal M.: CECAM Workshop: Dissipative Particle Dynamics: Addressing Deficiencies and Establishing New Frontiers. Mol. Simul. 35(9), 766-769 (2009).
5. Lísal M., Brennan J.K., Smith W.R.: Mesoscale Simulation of Polymer Reaction Equilibrium: Combining Dissipative Particle Dynamics with Reaction Ensemble Monte Carlo. II. Supramolecular Diblock Copolymers. J. Chem. Phys. 130(10), 104902-1 – 104902-15 (2009).
6. Malijevský A., Lísal M.: Density Functional Study of Chemical Reaction Equilibrium for Dimerization Reactions in Slit and Cylindrical Nanopores. J. Chem. Phys. 130(16), 164713-1-24 (2009).
7. Melnyk R., Nezbeda I., Henderson D., Trokhymchuk A.: On the Role of the Reference System in Perturbation Theory: An Augmented van der Waals Theory of Simple Fluids. Fluid Phase Equilib. 279(1), 1-10 (2009).

8. Morávková L., Wagner Z., Linek J.: Volumetric Behaviour of Binary Liquid Systems Composed of Toluene, Isooctane and Methyl tert-Butyl Ether at Temperatures from 298.15 K to 328.15 K. J. Chem. Thermodyn. 41(5), 591-597 (2009).
9. Moučka F., Nezbeda I.: Multi-particle Sampling in Monte-Carlo Simulations on Fluids: Efficiency and Extended Implementations. Mol. Simul. 35(8), 660–672 (2009).
10. Moučka F., Nezbeda I.: Partial Molar Volume of Methanol in Water: Effect of Polarizability. Collect. Czech. Chem. Commun. 74(4), 559-563 (2009).
11. Posel Z., Lísal M., Brennan J.K.: Interplay Between Microscopic and Macroscopic Phase Separations in Ternary Polymer Melts: Insight from Mesoscale Modelling. Fluid Phase Equilib. 283(1-2), 38-48 (2009).
12. Rouha M., Nezbeda I.: Fluids of Pseudo-Hard Bodies: From Simulations to Equations of State. Fluid Phase Equilib. 278(1-2), 15-19 (2009).
13. Rouha M., Nezbeda I.: Non-Lorentz–Berthelot Lennard-Jones Mixtures: A Systematic Study. Fluid Phase Equilib. 277(1), 42-48 (2009).
14. Škvor J., Nezbeda I.: Percolation Threshold Parameters of Fluids. Phys. Rev. E. 79(4), 041141-7 (2009).
15. 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, in press.
16. Maksimov M., Vlček L., Prokop A.: Development of Compartmental Tumor Uptatake and Organ Washout Model for Drug and Imaging Purposes: Retrospective Study. Mol. Pharmacol., submitted.
17. Mamontov E., Wesolowski D.J., Vlček L.: Dynamics of Hydration Water on Rutile Studied by Backscattering Neutron Spectroscopy. J. Phys. Chem. C, submitted.
18. Morávková L., Wagner Z., Linek J.: Volumetric Properties of Pyridine, 2-Picoline, 3-Picoline, and 4-Picoline at Temperatures from (298.15 to 328.15) K and at Pressures up to 40 MPa. J. Chem. Thermodyn. 42(1), 63-69 (2010).
19. Pavlíček J., Bogdanić G., Wichterle I.: Circulation Micro-Ebulliometer for Determination of Vapor–Liquid Equilibria. Fluid Phase Equilib., submitted.
20. Payne C.M., Zhao X., Vlček L., Cummings P.T.: Electrophoresis of Single-stranded DNA through Nanoelectrode Gaps from Molecular Dynamics: Impact of Gap Width. Phys. Rev. E., submitted.
21. Wagner Z.: Robust Method of Determination of Interaction Parameters of Equation of State from High Pressure Vapour-Liquid Equilibrium Data. Fluid Phase Equilib., submitted.

Books and monographs

22. Linek J.: Annual Report 2008. 79 pp., Ústav chemických procesů AV ČR, v. v. i., Praha 2009.
23. Bogdanić G., Wichterle I., Erceg Kuzmić A.: Collection of Miscibility Data and Phase Behavior of Binary Polymer Blends Based on Styrene, 2,6-Dimethyl-1,4-Phenylene Oxide and of Their Derivatives. 124 pp., Research Signpost, Trivandrum, in press.

International conferences

24. Aim K., Wichterle I.: Trans-esterification reaction coupled with vapour-liquid equilibrium in a quaternary system. 8th World Congress of Chemical Engineering (WCCE8), Abstract Book, p. 1138, Montréal, Quebec, Canada, 23-27 August 2009.
25. Bendová M., Aim K., Klusoň P., Sedláková Z., Černá I., Vašinová J.: Correlation of Liquid-Liquid Equilibria in Ternary Systems Containing Ionic Liquids. Thermodynamics 2009, Book of Abstracts, p. 41(21), London, Great Britain, 23-25 September 2009.
26. Bendová M., Klusoň P., Sedláková Z., Černá I., Vašinová J.: Liquid-Liquid Equilibrium in Ternary Systems 1-Chlorobutane + 1-Methylimidazole + Water / [bmim][PF6]. 9. Encontro Nacional de Química Física / 1st Iberian Meeting on Ionic Liquids, Book of Abstracts, p. 61, Aveiro, Portugal, 15-16 June 2009.
27. Bendová M., Wagner Z., Aim K.: Liquid-Liquid Equilibria in Systems 1-Ethyl-3-methyl-imidazolium Ethyl sulfate + C7-Hydrocarbons. 24th European Symposium on Applied Thermodynamics ESAT 2009, Book of Abstracts, pp. 325-326 (2 pp. full text on CD-ROM), Santiago de Compostela, Spain, 27 June - 01 July 2009.
28. Bogdanić G., Erceg Kuzmić A., Wichterle I.: Determination and Prediction of VLE Data in Polymer-Solvent Systems. Part 2. 24th European Symposium on Applied Thermodynamics ESAT 2009, Book of Abstracts, pp. 206-207 (2 pp. full text on CD-ROM), Santiago de Compostela, Spain, 27 June - 01 July 2009.

29. Bogdanić G., Wichterle I., Erceg Kuzmić A.: Modeliranje fizikalno-kemijskih svojstava nafte. (Cro). 34. Hrvatski salon inovacija s medunarodnim sudjelovanjem INOVA 2009, Katalog INOVA 2009, p. 79, Zagreb, Croatia, 11-15 November 2009.
30. Linek J., Morávková L., Wagner Z.: Volumetric Behaviour of Binary and Ternary Liquid Systems Composed of Toluene, Isooctane and Methyl tert-Butyl Ether at Temperatures from 298.15 K to 328.15 K. 24th European Symposium on Applied Thermodynamics, Book of Abstracts p. 305 (8 pp. full text on CD-ROM), Santiago de Compostela, Spain, 27 June - 01 July 2009.
31. Linek J., Morávková L., Wagner Z.: Volumetric Behaviour of Binary and Ternary Liquid Systems Composed of Toluene, Isooctane and Methyl tert-Butyl Ether at Temperatures from 298.15 K to 328.15 K. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 247 (6 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
32. Morávková L., Wagner Z., Linek J.: Volumetric Behaviour of Binary Liquid Systems Composed of Toluene, Isooctane and Methyl tert-Butyl Ether at Temperatures from 298.15 K to 328.15 K. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 201 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
33. Nezbeda I.: Problems of Molecular Theories of Fluid Mixtures: Intermolecular Potential Models and Combining Rules. 24th European Symposium on Applied Thermodynamics ESAT 2009, Book of Abstracts, p. 193, Santiago de Compostela, Spain, 27 June - 01 July 2009.
34. Nezbeda I.: Problems of Molecular Theories of Fluid Mixtures: Intermolecular Potential Models and Combining Rules. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 123, Srní, Šumava, Czech Republic, 19-22 October 2009.
35. Petrus P., Lísal M.: Self-Assembly of Symmetrical Diblock Copolymers in Nanopatterned Confinement: Insight from Dissipative Particle Dynamics Simulations. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 148, Tatranské Matliare, Slovakia, 25-29 May 2009.
36. Petrus P., Lísal M., Brennan J.K.: Self-Assembly of Symmetrical and Unsymmetrical Diblock Copolymers in Confinement: Insight from Dissipative Particle Dynamics Simulations. 24th European Symposium on Applied Thermodynamics ESAT 2009, Book of Abstracts, p. 35, Santiago de Compostela, Spain, 27 June - 01 July 2009.
37. Posel Z., Lísal M.: Interplay between Microscopic and Macroscopic Phase Separations In Ternary Polymer Melts: Insight from Mesoscale Modelling. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 147, Tatranské Matliare, Slovakia, 25-29 May 2009.
38. Předota M., Wesolowski D.J., Cummings P.T.: Molecular Simulations of Electrokinetics Phenomena at Solid-Liquid Interface. 24th European Symposium on Applied Thermodynamics ESAT 2009, Book of Abstracts, pp. 16-17 (2 pp. full text on CD-ROM), Santiago de Compostela, Spain, 27 June - 01 July 2009.
39. Rotrekl J., Sedláková Z., Bendová M., Vrbka P., Jacquemin J.: Solid - Liquid Equilibrium Measurements in Binary System N,N-diethylamine + [C2mim][Tf2N]. 24th European Symposium on Applied Thermodynamics, Book of Abstracts, pp. 333-334, Santiago de Compostela, Spain, 27 June - 01 July 2009.
40. Sedláková Z., Bendová M., Wagner Z., Jacquemin J.: High-pressure Measurements in Binary Systems Containing Supercritical CO_2. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 198 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
41. Smith W.R., Francová M., Jirsák J., Škvor J., Nezbeda I.: Molecular-level Simulation of Electrolyte Systems in the Cu-Cl Hydrogen Production Cycle. 8th World Congress of Chemical Engineering (WCCE8), Abstract Book, p. 430, Montréal, Quebec, Canada, 23-27 August 2009.
42. Smith W.R., Francová M., Kowalski M., Lísal M., Nezbeda I.: Molecular-level Simulation Methodology for Refrigerant Cycle Design Involving Refrigerant Mixtures. 8th World Congress of Chemical Engineering (WCCE8), Abstract Book, p. 430, Montréal, Quebec, Canada, 23-27 August 2009.
43. Smith W.R., Nezbeda I., Francová M., Jirsák J., Škvor J.: Molecular-level Simulation of Thermodynamics Properties of Aqueous Electrolyte Systems. 24th European Symposium on Applied Thermodynamics ESAT 2009, Book of Abstracts p. 44 (2 pp. full text on CD-ROM), Santiago de Compostela, Spain, 27 June - 01 July 2009.
44. Wagner Z., Schwarz J., Ždímal V., Eleftheriadis K., Lazaridis M., Smolík J.: Analysis of Time Evolution of Particle Size Distribution. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 116-119, Prague, Czech Republic, 10-14 August 2009.

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Fields of research

- Advanced catalytic oxidation processes
- Catalytic combustion of volatile organic compounds in waste gases
- Catalytic decomposition of N_2O
- Design of new theoretical models for structure-activity relationships
- Morphology and application properties of catalysts based on functional polymers
- Preparation of hierarchic nanomaterials
- Sulphide catalysts of unconventional composition
- Temperature programmed techniques in characterization of catalysts
- Texture of porous solids
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Transport processes in porous solids
- Unconventional preparation of supported molybdenum catalysts

Applied research

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

Research projects

Hydrogen oriented underground coal gasification for Europe
(O. Šolcová, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00006)

The project explores the technology for hydrogen production through underground gasification of coal in a dynamic geo-reactor. The process is controlled through purposed dynamic changes in temperature and pressure of the reactants and products. The project addresses CBM usage and CO_2 sequestration in coal deposits. The environmental fingerprint of the technology on air, water and strata stability is evaluated. The locations of demonstration plants are chosen through computer modelling and simulation. Large scale production of hydrogen from coal is crucial for coal mining industries and will serve the needs of energy, chemistry and transportation sectors of Europe. [Refs. 29, 35, 46, 47, 102, 108, 109]

Hierarchic nanosystems for microelectronics

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

Project develops the complex composite systems with precisely defined performance applicable in microelectronics. The individual components will be formed by small arranged particles which will ensure partial function inevitable for functioning of the whole system. These composite structures should be directly applicable as elements of special sensors, photoelectric energy sources, microelectrodes for analytic instruments etc. The general aim of the project is the accumulation of sufficient amount of high-quality experimental data to be applied for design and implementation of practical nanotechnologies. Professionally, the project is focused on the study of preparation of hierarchic nanostructures, inclusive the structural and functional characterization, as well as on prediction of properties by means of mathematical modeling. [Refs.7, 18, 19, 42, 57, 61, 90, 91, 96, 97]

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

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

Project deals with development and optimization of extraction technique for purification and total crystallization prepared oxidic materials with high-ordered mesoporous structure. Developed extraction technique using fluids in supercritical and subcritical state 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 microelectronic will be synthesized by templating using amphiphilic and ionic surfactants in aqueous and alcoholic solution with metal chloride and alkoxide. [Refs. 45, 94, 95]

Advanced photocatalytic processes - nanotechnology for environmental

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

This project will focused on preparation and characterization of specially designed photoactive materials and their utilization for decomposition of a large series of potential water contaminants ranging from phenols, chlorinated phenols, polybrominated diphenyl ethers and alcohols to herbicides, pesticides, pharmaceuticals, industrial colorants, pigments and dyes. The special focus will be devoted to design of the reactor system; selectively prepared photoactive nanostructures together with design of effective photoreactors including

mathematical modelling of involved physical and chemical processes and generalization of obtained results. [Refs. 16, 21, 59, 82, 83, 92, 98]

Synergistic effects in hydrodesulfurization and oxidation reactions

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

12-Tungstophosphoric heteropolyacid and SBA-15 as a support were used to prepare catalysts for hydrodesulfurization (HDS) of thiophene. Their physical-chemical and catalytic properties were examined. The effect of other novel supports like mesoporous titanate nanotubes and titania-zirconia nanostructured materials on the properties of the HDS catalysts was studied. [Refs. 28, 64, 88, 101]

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

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

Formation of LDH precursors on an oxidized Al foil, a model of structured catalyst supports, under hydrothermal conditions was studied in detail. After calcination, catalytic activity of corresponding metal oxides was examined. The effect of LDH precursor crystallinity was studied over the Ni_4Al_2 system. The highest catalytic activity was found with the system not having too high crystallinity. The effect of various promoters and the mode of their incorporation into the Co_4MnAl oxidation catalyst (prepared by coprecipitation) and their effect on the activity and selectivity in total oxidation of model VOC (toluene, ethanol) were studied in detail. Among the promoters studied addition of potassium showed the highest positive effect on catalyst activity, as it modifies acid-base properties of the catalysts. [Refs. 13, 22, 23, 66, 67, 74, 75, 85-87]

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

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

The effect of alkali addition to the calcined Co_4MnAl-LDH like compounds on the catalyst activity in decomposition of N_2O was studied, as well as stability of the catalyst in the presence of real reaction mixture (containing H_2O, O_2 and NO_x). Pelleting pressure of the coprecipitated LDH of transition metals studied in a wide range of pressures showed that pelleting under the pressure of 6 MPa provides sufficiently hard pellets and does not influence catalytic activity. The use of Co_4MnAl catalyst in N_2O decomposition was patented. [Refs. 9, 27, 56, 79, 80, 100]

Advanced catalytic processes and materials

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

The concerted project is aimed at a development of 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. The processes in question are stereoselective and regioselective transformations on chiral catalytic centers and processes with significant environmental impact. Coordination of Thesis projects is planned in the field of catalysis, e.g., developed Rh catalysts can be tested in stereospecific polymerizations (CU), asymmetric synthesis (ICT) and hydrocarbonylations; oxidation catalysts can be tested in organic synthesis (ICT, UPa, ICPF), oxidation polymerization (CU) and synthesis of chemical

specialties (JH IPC); new mesoporous materials prepared at JH IPC will be used in all other partner laboratories, etc. [Refs. 20, 26, 39, 58 , 84, 89, 120]

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

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

Aromatic polyimides (PI) exhibit very good chemical and mechanical stability up to 250 ºC. They also exhibit a high selectivity for membrane separation of small molecules as hydrogen. The main drawback PI membranes preventing their wide application, e.g. in membrane reactors is a very low species flow. The principal goal of the project is thus, enhancement of species flow without essential deterioration of the selectivity. The approaches considered to enhance species flow through membranes are: (i) thinning of the PI layer upon introducing porous supports or armour, (ii) formation of PI layer upon radial stress, (iii) producing local stress fields by introducing inclusions, (iv) introducing porous inclusions at concentrations near to percolation threshold. To optimize two-phase membrane composition, it is intended to perform a rigorous treatment of mass transport in composite media using image analysis together with computer experiment. [Refs. 4, 5, 8, 51, 62, 63, 65, 70]

Modern theoretical methods for the analysis of chemical bonding

(R. Ponec, supported by GACR grant No. GA203/09/118)

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. 3, 6, 24, 30-33, 49]

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

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

Mesoporous silica-alumina dealuminated to different degrees was studied as a support for Pt catalysts. Dealumination led to substantially higher surface area and acidity of supports, and consequently to better activity of Pt catalysts in hydrodesulfurization (HDS) of thiophene (TH). Mesoporous alumina was also studied as support for Co Mo catalysts. These catalysts showed better activity in HDS of TH and benzothiophene (BT), due to about twofold BET surface area over common industrial aluminas. A slurry impregnation method was studied in syntheses of alumina supported Ni Mo catalysts and their catalytic properties were evaluated in BT HDS. HDS of TH and its inhibition by pyridine (PY) was studied on noble metal promoted (Rh, Ru) Mo/alumina catalysts. These catalysts showed high nitrogen tolerance and consequently, in the presence of PY better HDS activities in comparison to conventional Mo and Co Mo catalysts. [Refs. 11, 15, 68, 76-78, 117, 118]

Functional macroreticular polymers as catalyst carriers
(K. Jeřábek, joint project with Department of Chemical Sciences, University of Padua, Italy, supported by ASCR, grant No. M200720902)

In the project, polymer-based catalysts bearing either covalently bonded acidic groups and/or metal nanoparticles are investigated. Using combination of various physico-chemical methods, morphology and steric conditions in polymeric catalysts of both laboratory and commercial origin has been examined. Methods for modification of porous structure of functional polymers by additional postpolymerization cross-linking were also studied. In starting stages is the investigation of modification of chemical nature of polymer catalyst carriers for applications in highly lipophilic environment. [Refs. 1, 2, 34, 48, 73]

Porosity investigations of polyHIPEs using ISEC methods
(K. Jeřábek, joint project with Faculty of Chemistry and Chemical Engineering, University of Maribor, Slovenia, supported by MEYS, KONTAKT project No. MEB 090811)

High internal phase emulsions (HIPE) can be used as templates for porous reactive monolithic polymers. Morphological structure of emulsion derived polymers was studied in their swollen state using inverse steric exclusion chromatography. [Ref. 69]

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

The aim of this work is to compare peculiarities of Cl-VOC (also CVOC) and S-VOC removal from air over catalysts containing noble metals stabilized by different supports. Nano-gold containing catalysts attracted the special attention due to Au^0 stability in oxidative atmosphere and its resistance towards SO_x and HCl formed. $(Au+Rh)/TiO_2$ demonstrated efficient and stable S-VOC and Cl-VOC removal at T = 260 – 320 °C and high specific gas velocity, the residual amount of pollutants can be reduced to < 10 ppm. Efficiency and stability of the nano-gold containing catalysts is compared with Pd-containing samples on different supports, as well as $CuO\text{-}MnO_2$ mixed oxide (known as an active catalyst for VOC oxidation). [Refs. 66, 67]

Reactive chemical barriers for decontamination of heavily polluted waters
(P. Klusoň, joint project with Dekonta a.s., supported by MIT, grant No. FR-TI1/065)

The project aims for the practical development of special oxidation processes used for decontamination of industrially polluted subsurface waters. The used methods are: photocatalytic oxidation with titanium dioxide, photocatalytic oxidation with synthetic porphyrines and oxidations with various organic peroxides and hydrogen peroxide. The project deals in a complex manner with the problem of industrial pollution with a range of organic chemicals at concentrations and the area scale that can hardly be treated in any other way. The Recheba concept represents a kind of passive approach, however, assisted with highly advanced processes for effective water decontamination. The systems are now tested on a laboratory scale, in parallel they will be modified and scaled-up for practical testing on three selected industrial sites. The efficiencies of the chosen methodologies will be compared and the most suitable one will be implemented to the final form that will be produced and long-term tested. [Refs. 113, 114]

Advanced catalytic reactions for fine chemicals
(P. Klusoň, bilateral project with University of Szeged, Department of Chemsirty, Hungary, project KONTAKT No. MEB 040802, MEYS)

This project was (in 2009) focused on the study of different immobilization methods. Based on the results obtained under homogeneous conditions, Fe(phthalocyanine) was selected as a suitable candidate for immobilization. The homogeneous results showed this complex to be the most active one, among the different Me(phthalocyanine)s for the non-photocatalytic oxidation. For the heterogenization we have applied first the Augustine method, namely to anchore the complex by heteropoly-acid. For the characterization we have used the XRD and FT-IR spectroscopy. Second way of immobilization was the preparation of a "ship-in-a-bottle" type catalyst. The prepared catalyst was active in the oxidation of 4-chlorophenol, even the activity was a little bit smaller than activity of the homogeneous analogue. However the heterogenized catalyst was easy to handle and because of its reusability its practical application is still advantageous. [Ref. 17]

Composed molecular templates for preparation of assembled functional nanoparticles
(P. Klusoň, bilateral project with Bangor University, School of Chemistry, Wales, UK, supported by ASCR, grant No. M200720904)

To emulate at least some of the effectiveness of NATURE in making smart functional structures and systems man has had to develop many different empirical and later also scientific concepts. Currently such attempts are reflected in the steep growth of interest in nanoscience and nanotechnologies. Although there has already been much progress in the synthesis, assembly and fabrication of nanomaterials, their potential applications in a wider range of practical technologies are still rare. These new technologies are expected to have an impact on chemistry, energy production, energy storage, electronics, machinery, aircrafts, space exploration, environment protection, etc. Independently of types of new materials (or their application), one of the most important points concerns chemical (or physical) pathways that are capable to yield them. Among the suitable methods, bottom-up approaches involving templates have dominated for the preparation of one-dimensional or multidimensional nanostructures. This pathway is particularly useful if precise replication is achieved in the nanometer precision. It corresponds to the assembly of well-defined nanobuilding blocks consisting of perfectly calibrated objects keeping their integrity in the final material. [Refs. 25, 44, 60, 99]

Utilization of combined thermal desorption and catalytic oxidation methods for solid waste decontamination
(O. Šolcová, joint project with Dekonta, a.s., supported by MIT, grant No. FR-TI1/059)

Project develops and verifies a new technology for decontamination of solid waste containing toxic organic substances, which is based on treatment of 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. [Refs. 52-54, 111, 115, 116]

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, Sofia, Bulgaria: Synergistic effects in hydrodesulfurization and oxidation reactions
University of Helsinki, Helsinki, Finland: Structure and bonding in metal carbonyls
University of Oulu, Oulu, Finland: New catalysts for VOC oxidation
European Membrane Institute, Montpellier, France: Synthetic porphyrites
University of Paris VI, Paris, France: Theory of chemical bond
University of Poitiers, Poitiers, France: New catalysts for VOC elimination
University of Stuttgart, Stuttgart, Germany: Transport characteristics for coal gasification
University of Szeged, Szeged, Hungary: Homogenous catalytic complexes on surface of heterogeneous matrix
Chemical Institute of Hungarian Academy of Sciences, Budapest, Hungary: Structure and bonding in metal carbonyls
Instituto di Scienze e Tecnologie Molecolari del CNR et Universita di Milano, Milano, Italy: Structure and bonding in metal carbonyls
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
Institute of Computational Chemistry, University of Girona, Girona, Spain: Theory of chemical bond
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

Visitors

B. Corain, University of Padua, Italy
D. L. Cooper, University of Liverpool, UK
P. Krajnc, University of Maribor, Slovenia

Teaching

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

Publications

Original papers

1. Centomo P., Zecca M., Králik M., Gasparovičová D., Jeřábek K., Canton P., Corain B.: Cross-linked Poly-vinyl Polymers versus Polyureas as Designed Supports for Catalytically Active M^0 Nanoclusters Part II. Pd^0/Cross-linked Poly-vinyl Polymers versus Pd^0/EnCat^{TM}30NP in Mild Hydrogenation Reactions. J. Mol. Catal. A-Chem. 300(1-2), 48-58 (2009).
2. Centomo P., Zecca M., Zoleo A., Maniero A.L., Canton P., Jeřábek K., Corain B.: Cross-linked Polyvinyl Polymers versur Polyureas as Designed Supports for Catalytically Active M^0 Nanoclusters. Part III. Nanometer Scale Structure of the Cross-linked Polyurea Support EnCat 30 and of the Pd^{II}/EnCat 30 and Pd^0/EnCat 30NP Catalysts. Phys. Chem. Chem. Phys. 11, 4068-4076 (2009).
3. Cooper D.L., Ponec R.: Anatomy of Bond Formation: Insights from the Analysis of Domain-Averaged Fermi Holes in Momentum Space. Int. J. Quantum Chem. 109(11), 2383-2392 (2009).
4. Čapek P., Hejtmánek V., Brabec L., Zikánová A., Kočiřík M.: Stochastic Reconstruction of Particulate Media Using Simulated Annealing: Improving Pore Connectivity. Transp. Porous Media 76(2), 179-198 (2009).
5. Čapek P., Hejtmánek V., Brabec L., Zikánová A., Kočiřík M., Bernauer B.: 3D Stochastic Replicas of Porous Solids: A Way to Improve Predicted Diffusivity. Diffusion Fundamentals 11(79), 1-2 (2009).
6. Durdevič J., Gutman I., Ponec R.: Verifying the PCP-rule by Five-Center Bond Indices. J. Serb. Chem. Soc. 74(5), 549-554 (2009).
7. Floriš T., Klusoň P., Bartek L., Pelantová H.: Quaternary Ammonium Ionic Liquids for Immobilization of Chiral Ru-BINAP Complexes in Asymmetric Hydrogenation of β-Ketoesters. Appl. Catal., A 366(1), 160-165 (2009).
8. Fryčová M., Sysel P., Hrabánek P., Kočiřík M, Brabec L., Zikánová A., Barnauer B., Čapek P., Hejtmánek V.: Helium Permeation through Mixed Matrix Membranes Based on Polyimides and Silicalite-1. Diffusion-fundamentals.org 11(6), 1-2 (2009).
9. Galejová K., Obalová L., Jirátová K., Pacultová K., Kovanda F.: N_2O Catalytic Decomposition - Effect of Pelleting Pressure on Activity of Co-Mn-Al Mixed Oxide Catalyst. Chem. Pap. 63(2), 172-179 (2009).
10. Gulková D., Kaluža L., Vít Z., Zdražil M.: Support Effect in Hydrodesulfurization over Ruthenium Sulfide. Petroleum and Coal 51(2), 146-149 (2009).
11. Gulková D., Yoshimura Y., Vít Z.: Mesoporous Silica-Alumina as Support for Pt and Pt-Mo Sulfide Catalysts; Effect of Pt Loading on Activity and Selectivity in HDS and HDN of Model Compounds. Appl. Catal., B 87(3-4), 171-180 (2009).
12. Hejtmánek V., Čapek P., Brabec L., Zikánová A., Kočiřík M.: Určování mikrostrukturních deskriptorů z digitálních snímků pórovitých látek. (Czech) Determination of Microstructure Descriptors from Digital Images of Porous Media. Chem. Listy 103(6), 496-502 (2009).
13. Jirátová K., Mikulová J., Klempa J., Grygar T., Bastl Z., Kovanda F.: Modification of Co-Mn-Al Mixed Oxide with Potassium and Its Effect on Deep Oxidation of VOC. Appl. Catal., A 361(1-2), 106-116 (2009).
14. Kaluža L., Zdražil M.: Slurry Impregnation of ZrO_2 Extrudates: Controlled Eggshell Distribution of MoO_3, Hydrodesulfurization Activity, Promotion by Co. Catal. Lett. 127(3-4), 368-376 (2009).
15. Kaluža L., Zdražil M., Vít Z.: Deposition of NiO onto MoO_3/gamma-Al_2O_3 Extrudates by Slurry Impregnation Method. Reac. Kinet. Catal. Lett. 97(2), 307-313 (2009).
16. Klusoň P., Drobek M., Kalaji A., Karásková M., Rakušan J.: Preparation, Chemical Modification and Absorption Properties of Various Phthalocyanines. Res. Chem. Intermed. 35(1), 103-116 (2009).
17. Klusoň P., Drobek M., Zsigmond A., Baranyi J., Bata P., Zárubová Š., Kalaji A.: Environmentally Friendly Phthalocyanine Catalysts for Water Decontamination - Non Photocatalytic Systems. Appl. Catal. B-Environ. 91(3-4), 605-609 (2009).
18. Kment Š., Klusoň P., Drobek M., Kužel R., Kohout M., Hubička Z.: Preparation of Thin Phthalocyanine Layers and Their Structural and Absorption Properties. Thin Solid Films 517(17), 5274-5279 (2009).
19. Kment Š., Klusoň P., Straňák V., Virostko P., Krýsa J., Čada M., Stateva R.S., Kohout M., Morozová M., Adámek P., Hubička Z.: Photo-induced Electrochemical Functionality of the TiO_2 Nanoscale Coatings. Electrochim. Acta 54(12), 3352-3359 (2009).
20. Kment Š., Klusoň P., Žabová H., Churpita A., Chichina M., Čada M., Gregora I., Krýsa J., Hubička Z.: Atmospheric Pressure Barrier Torch Discharge and its Optimization for Flexible Deposition of TiO_2 Thin Coatings on Various Surfaces. Surf. Coat. Technol. 204(5), 667-675 (2009).
21. Kočí K., Obalová L., Matějová L., Plachá D., Lacný A., Jirkovský J., Šolcová O.: Effect of TiO_2 Particle Size on the Photocatalytic Reduction of CO_2. Appl. Catal., B 89(3-4), 494-502 (2009).

22. Kovanda F., Mašátová P., Novotná P., Jirátová K.: Formation of Layered Double Hydroxides on Alumina Surface in Aqueous Solutions Containing Divalent Metal Cations. Clay Clay Miner. 57(4), 425-432 (2009).
23. Kovanda F., Rojka T., Bezdička P., Jirátová K., Obalová L., Pacultová K., Bastl Z., Grygar T.: Effect of Hydrothermal Treatment on Properties of Ni-Al Layered Double Hydroxides and Related Mixed Oxides. J. Sol. State Chem. 182(1), 27-36 (2009).
24. Mandado M., Ponec R.: Electron Reorganization in Allowed and Forbidden Reactions: Multicenter Bond Indices as a Measure of Aromaticity and/or Anti-aromaticity in Transition States of Pericyclic Electrocyclizations. J. Phys. Org. Chem. 22(12), 1225-1232 (2009).
25. Mason S., Holliman P., Kalaji M., Klusoň P.: The Production of Nanoparticulate Ceria Using Reverse Micelle Sol-Gel Techniques. J. Mater. Chem. 19(21), 3517-3522 (2009).
26. Morozová M., Klusoň P., Krýsa J., Zlámal M., Šolcová O., Kment Š., Steck T.: Role of the Template Molecular Structure on the Photoelectrochemical Functionality of the Sol–Gel Titania Thin Films. J. Sol-Gel Sci. Technol. 52(3), 398-407 (2009).
27. Obalová L., Karásková K., Jirátová K., Kovanda F.: Effect of Potassium in Calcined Co-Mn-Al Layered Double Hydroxide on the Catalytic Decomposition of N_2O. Appl. Catal., B 90(1-2), 132-140 (2009).
28. Palcheva R., Spojakina A.A., Dimitrov L., Jirátová K.: Heteropolyacid Supported on Modified SBA-15 as Catalyst in HDS of Thiophene. Micropor. Mesopor. Mat. 122(1-3), 128-134 (2009).
29. Petráš D., Kimmer D., Soukup K., Klusoň P.: Bezpečná nanovlákna. (Czech) Safe Nanofibers. Chem. Listy 103(12), 1009-1016 (2009).
30. Ponec R., Feixas F: Domain Averaged Fermi Hole Analysis for Open-Shell Systems. J. Phys. Chem. A 113(19), 5773-5779 (2009).
31. Ponec R., Feixas F.: Peculiarites of Multiple Cr-Cr Bonding. Insights from the Analysis of Domain Averaged Fermi holes. J. Phys. Chem. A 113(29), 8394-8400 (2009).
32. Ponec R., Fias S., Van Damme S., Bultinck P., Gutman I., Stanković S.: The Close Relation between Cyclic Delocalization, Energy Effects of Cycles and Aromaticity. Collect. Czech. Chem. Commun. 74(1), 147-166 (2009).
33. Ponec R., Gatti C.: Do the Structural Changes Defined by the Electron Density Topology Necessarily Affect the Picture of the Bonding?. Inorg. Chem. 48(23), 11024-11031 (2009).
34. Soukupová K., Sassi A., Jeřábek K.: Reinforcing of Expanded Polymer Morphology Using Peroxy Radical Initiator. React. Funct. Polym. 69(6), 353-357 (2009).
35. Šolcová O., Soukup K., Rogut J., Stanczyk K., Schneider P.: Gas Transport Through Porous Strata from Underground Reaction Source; the Influence of the Gas Kind, Temperature and Transport-Pore Size. Fuel Process. Technol. 90(12), 1495-1501 (2009).
36. Žabová H., Církva V.: Microwave Photocatalysis III. Transition Metal Ion-Doped TiO_2 Thin Films on Mercury Electrodeless Discharge Lamps: Preparation, Characterization and Their Effect on the Photocatalytic Degradation of Mono-Chloroacetic Acid and Rhodamine B. J. Chem. Technol. Biotechnol. 84(11), 1624-1630 (2009).
37. Žabová H., Církva V., Hájek M.: Microwave Photocatalysis II: Novel Continuous-Flow Microwave Photocatalytic Experimental Set-up with Titania-Coated Mercury Electrodeless Discharge Lamps. J. Chem. Technol. Biotechnol. 84(8), 1125-1129 (2009).
38. Žabová H., Dvořák B.: Gas Phase Degradation of Acetone Using a TiO_2 Photocatalyst Supported on a Polyester Fabric. Reac. Kinet. Catal. Lett. 98(1), 165-175 (2009).
39. Žabová H., Sobek J., Církva V., Šolcová O., Kment Š., Hájek M.: Efficient Preparation of Nanocrystalline Anatase TiO_2 and V/TiO_2 Thin Layers Using Microwave Drying and/or Microwave Calcination Technique. J. Solid. State Chem. 182(12), 3387-3392 (2009).
40. Kaštánek F., Kaštánek P., Maléterová Y.: Dechlorination of PCBs in Aqueous Mixtures with Zero-Valent Iron in Statu Nascendi. Influence of Microwaves on the Rate of Reaction. J. Hazard. Mater., submitted.
41. Kaštánek P., Kaštánek F., Hájek M.: Microwave-enhanced Thermal Adsorption of Polyhalogenated Biphenyls from Contaminated Soil. J. Hazard. Mater., submitted.
42. Kment Š., Klusoň P., Hubička Z., Krýsa J., Čada M., Gregora I., Deyneka A., Remes Z., Žabová H., Jastrabík L.: Double Hollow Cathode Plasma Jet -Low Temperature Method for the TiO_2-xN_x Photoresponding Films. Electrochim. Acta, in press.
43. Kubička D., Kaluža L.: Deoxygenation of Vegetable Oils over Sulfided Ni, Mo and Ni Mo Catalysts. Appl. Catal., A 372(2), 199-208 (2010).
44. Lutecki M., Šolcová O., Werner S., Breitkopf C.: Synthesis and Characterization of Nanostructured Sulfated Zirconias. J. Sol-Gel Sci. Technol., in press.
45. Matějová L., Cajthaml T., Matěj Z., Benada O., Klusoň P., Šolcová O.: Super/Subcritical Fluid Extractions for Preparation of the Crystalline Titania. J. Supercrit. Fluids, in press.

46. Soukup K., Petráš D., Klusoň P., Šolcová O.: Nanofiber Membranes—Evaluation of Gas Transport. Catal. Today, submitted.
47. Soukup K., Rogut J., Ludwik-Pardała M., Wiatowski M., Grabowski J., Schneider P., Šolcová O.: Porous Fe_2O_3/Al_2O_3 and Fe/Al_2O_3 Pellets for Hydrogen Storage: Texture and Transport Characteristics. Int. J. Hydrog. Energy, submitted.
48. Soukupová K., Sassi A., Jeřábek K.: Modifications in the Morphology of Poly(styrene-co-divinylbenzenes) Induced by Gamma-ray Irradiation. React. Funct. Polym., submitted.

Books and monographs

49. Bultinck P., Fias S., Mandado M., Ponec R.: Correlation between Electron Delocalization and Ring Currents in All Metallic. CRC Press, in press.

Chapters in books

50. Církva V., Žabová H.: Thin Nanoporous Titania Films on the Electrodeless Discharge Lamps for Photocatalysis. In: Handbook of Photocatalysts: Preparation, Structure and Applications. (Castello, G.K., Ed.), Nova Science Publishers, in press.
51. Čapek P., Hejtmánek V.: A Relationship between Pore Shapes and Mercury Porosimetry Curves as Revealed by a Random Pore Networks. In: Characterisation of Porous Solids VIII. (Kaskel, S., Ed.), pp. 385-393, RSC Publishing, Cambridge 2009.
52. Šolcová O., Matějová L., Hudec P., Schneider P.: Modified BET Equation for Determination of Micropore Pore Volume and Mesopore Surface Area in Microporous-Mesoporous Solids. In: Characterisation of Porous Solids VIII. (Kaskel, S., Ed.), pp. 218-224, RSC Publishing, Cambridge 2009.
53. Topka P., Zub Y.L., Karban J., Šolcová O.: Designing (Al-)SBA-15 Catalyst Pellet with Unique Properties. In: Characterisation of Porous Solids VIII. (Kaskel, S., Ed.), pp. 287-294, RSC Publishing, Cambridge 2009.
54. Šyc M., Pekárek V., Novák P., Šolcová O., Pohořelý M., Punčochář M., Ocelka T.: Fly Ash Properties, Disposal, and Treatment in Modernized Waste Incineration Plant with Catalytic Filter. In: Fly Ash: Reuse, Environmental Problems and Related Issues. (Telone, P.H., Ed.), Nova Science Publishers, New York, in press.

Patents

55. Jirátová K., Matoušek P., Markvart M.: Způsob odstranění thalia z kamence amonnohlinitého. (Czech) Removal of Thallium from Ammonium Aluminium Sulfate. Pat. No. PV 2007-443/CZ 300 285. Applied: 07.07.02, Patented: 09.03.02.
56. Obalová L., Jirátová K., Kovanda F.: Oxidický katalyzátor, zejména pro odstraňování N2O z odpadních plynů. (Czech) Oxide Catalyst, Especially for N_2O Removal from Waste Gases. Pat. No. PV 2007-583/CZ 300 807. Applied: 07.08.24, Patented: 09.08.12.
57. Šolcová O., Matějová L., Klusoň P., Cajthaml T.: Způsob přípravy krystalické formy oxidu titaničitého. (Czech) Preparation of TiO_2 Crystalline Phase. Pat. No. PV 2008-400. Applied: 08.06.25.
58. Šolcová O., Matějová L., Matěj Z.: Způsob přípravy oxidu titaničitého. (Czech) Method of Titania Preparation. Pat. No. PV 2008-326. Applied: 08.05.27.
59. Šolcová O., Topka P., Soukup K.: Způsob přípravy a regenerace pelet z křemičitanových a hlinitokřemičitanových mesoporézních molekulových sít a pelety připravené tímto způsobem. (Czech) Method of Pellet Preparation from Siliceous and Aluminosiliceous Mesoporous Molecular Sieves Including Regeneration and Pellets Prepared by this Method. Pat. No. PV 2008-325. Applied: 08.05.27.

International conferences

60. Bendová M., Aim K., Klusoň P., Sedláková Z., Černá I., Vašinová J.: Correlation of Liquid-Liquid Equilibria in Ternary Systems Containing Ionic Liquids. Thermodynamics 2009, Book of Abstracts, p. 41(21), London, Great Britain, 23-25 September 2009.
61. Bendová M., Klusoň P., Sedláková Z., Černá I., Vašinová J.: Liquid-liquid Equilibrium in Ternary Systems 1-Chlorobutane + 1-Methylimidazole + Water / [bmim][PF6]. 9. Encontro Nacional de Química Física / 1st Iberian Meeting on Ionic Liquids, Book of Abstracts, p. 61, Aveiro, Portugal, 15-16 June 2009.

62. Čapek P., Hejtmánek V., Brabec L., Zikánová A., Kočiřík M., Bernauer B.: 3D Stochastic Replicas of Porous Solids: A way to Improve Predicted Diffusivity. Diffusion Fundamentals III., Book of Abstracts, pp. 467-468, Athens, Greece, 23-26 August 2009.
63. Čapek P., Hejtmánek V., Brabec L., Zikánová A., Kočiřík M.: Pokroky ve stochastické rekonstrukci mikrostruktury pórovitých látek metodou simulovaného ochlazování. (Czech) Advances in Stochastic Reconstruction of Porous Solid Microstructure by the Method of Simulated Annealing. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 132 (17 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
64. Dimitrov L., Palcheva R., Spojakina A.A., Jirátová K.: Ni W Hydrodesulfurization Catalysts Supported on Mesoporous Titanate Nanotubes. 3rd International Symposium Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 129, Albena, Bulgaria, 06-09 September 2009.
65. Fryčová M., Sysel P., Hrabánek P., Kočiřík M., Brabec L., Zikánová A., Barnauer B., Čapek P., Hejtmánek V.: Helium Permeation Through Mixed Matrix Membranes Based Polyimides and Silicalite-1. Diffusion Fundamentals III, Book of Abstracts, pp. 124-125, Athens, Greece, 23-26 August 2009.
66. Gaálová J., Jirátová K.: Effect of Uranium in Co-Mn-Al Mixed Oxide Catalyst on Deep Oxidation of VOC. NANOISRAEL 2009, Abstracts, 325, Jerusalem, Israel, 30-31 March 2009.
67. Gaálová J., Jirátová K., Mikulová Z.: Co-Mn-Al-O Catalysts for Oxidation of VOC: Effect of Promoter. 2nd European Conference on Environmental Applications of Advanced Oxidation Processes, Proceedings, 6 pp. full text on CD-ROM, Nicosia, Cyprus, 09-11 September 2009.
68. Gulková D., Vít Z., Kaluža L., Zdražil M.: Dealuminated Mesoporous Silica-Alumina as Carrier for Pt Catalysts. 3th Czech-Italian-Spanish Trilateral Meeting on Catalysis and Micro/Meso-Porous Materials (CIS-3), Book of Abstracts, p. P10, Acireale, Sicily, Italy, 21-25 June 2009.
69. Hanková L., Pulko I., Krajnc P., Jeřábek K.: Porogenic Solvents Influence on Morphology of 4-Vinylbenzyl Chloride Based Polyhipes. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 292 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
70. Hejtmánek V., Čapek P., Brabec L.: Image Processing for the Purpose of 3D Reconstruction of Porous Membrane Support. 19th Annual Meeting of the North American Membrane Society, Programme, Poster 29, Charleston, South Carolina, USA, 20-24 June 2009.
71. Jandová J., Kaštánek F., Vu H.N., Štěpánek R., Maléterová Y., Šolcová O.: Comparison of Efficiency of Catalytic Reductive Dehalogenation of Polyhalogenated Compounds (PCBs, PBDE) in Aqueous Solutions with Selected Bimetallic Catalysts: Fe/Pd, Zn/Pd, Ni/Pd, Al/Pd, Mg/Pd. Catalytic Reactions Conference 2009, Poster Abstracts, p. 8, Antigua and Barbuda, 04-07 March 2009.
72. Jeřábek K.: Polymer-Supported Catalysts - a Bridge between Solid and Liquid Phase. Catalytic Reactions Conference 2009, Poster Abstracts, p. 11, Antigua and Barbuda, 04-07 March 2009.
73. Jeřábek K., Holub L.: Working-State Morphology of Ion Exchanger Catalysts and its Influence on Reaction Kinetics. 41st Symposium on Catalysis, Program Book of Abstracts, p. 15, Prague, Czech Republic, 02-03 November 2009.
74. Jirátová K., Gaálová J., Klempa J., Grygar T., Obalová L., Kovanda F.: Physical-Chemical Properties of Co-Mn-Al Mixed Oxide Modified with Potassium. 3th Czech-Italian-Spanish Trilateral Meeting on Catalysis and Micro/Meso-Porous Materials (CIS-3), Book of Abstracts, p. P14, Acireale, Sicily, Italy, 21-25 June 2009.
75. Jirátová K., Kovanda F., Klempa J., Ludvíková J., Krúpa L., Gaálová J.: Activity of Transition Metal Mixed Oxides Composited on Al_2O_3/Al Support in Total Oxidation on VOC. 41st Symposium on Catalysis, Program Book of Abstracts, pp. 68-69, Prague, Czech Republic, 02-03 November 2009.
76. Kaluža L., Gulková D., Šolcová O., Žilková N., Čejka J.: Promotional Effects of Co and Ni on the Hydrodesulfurization and Hydrodenitrogenation Activity of Mo Catalysts Supported on Organized Mesoporous Alumina. EuropaCat IX: "Catalysis for Sustainable World", Abstracts, p. 329 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
77. Kaluža L., Vít Z., Zdražil M.: Support Effect in Hydrodesulfurization of Thiophene over Rhodium Sulfide. 41. Symposium on Catalysis, Program Book of Abstracts, pp. 74-75, Prague, Czech Republic, 02-03 November 2009.
78. Kaluža L., Zdražil M., Vít Z.: Deposition of NiO onto MoO_3/gamma-Al_2O_3 Extrudates by Water-Assisted Spreading Method. 41st Symposium on Catalysis, Program Book of Abstracts, pp. 70-71, Prague, Czech Republic, 02-03 November 2009.
79. Karásková K., Obalová L., Jirátová K., Kovanda F.: Effect of Alkali Metals in Calcined Co-Mn-Al Layered Double Hydroxide on Catalytic Decomposition of N_2O. Catalytic Reactions Conference 2009, Poster Presentations, p. 19, Antigua and Barbuda, 04-07 March 2009.

80. Karásková K., Obalová L., Jirátová K., Kovanda F.: Effect of Promoters in Calcined Co-Mn-Al Layered Double Hydroxide on Catalytic Decomposition of N_2O. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 297 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
81. Kaštánek F., Braniyková I., Maléterová Y., Kaštánek P.: Využití destilačního odpadu v sekvenci bioplyn-kogenerace-produkce řas. (Czech) Utilization of Distillery Effluents and Agriculture Waste in a Biomas-Cogeneration-Microalgae Sequence. Seminář Biopaliva v dopravě , Book of Abstracts, 9 pp. full text on CD-ROM, Bratislava, Slovakia, 21-22 September 2009.
82. Kaštánek F., Maléterová Y., Šolcová O.: Catalytic Destruction of PCBs Dissolved in Aqueous and Oily Solutions. Influence of Microwaves on the Rate of Reaction. Catalytic Reactions Conference 2009, Poster Abstracts, p. 17, Antigua and Barbuda, 04-07 March 2009.
83. Kaštánek P., Kaštánek F., Hájek M., Sobek J., Šolcová O.: Dechlorination of Polychlorinated Bihphenyl (PCB) in Contaminated Soils and Oils. 11th International Conference on Environmental Science and Technology - CEST 2009, Volume of Abstracts, p. 76, Chania, Kréta, Greece, 03-05 September 2009.
84. Klusoň P., Floriš T.: Asymetrické hydrogenační reakce. (Czech) Asymmetric Hydrogenation Reactions. 56. Konference chemického a procesního inženýrství CHISA 20, Sborník, p. 29 (3 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
85. Kovanda F., Jirátová K., Koloušek D., Klempa J., Gaálová J.: Layered Double Hydroxide-Related Mixed Oxides Deposited on Al_2O_3/Al Support. EuropaCat IX: "Catalysis for Sustainable World", Abstracts, p. 536 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
86. Kovanda F., Koloušek D., Gaálová J., Jirátová K.: Příprava strukturovaných katalyzátorů depozicí podvojných vrstevnatých hydroxidů na kovový nosič. (Czech) Preparation of Structured LDHs over Metal Support. 61. Zjazd chemikov, ChemZi 5/9 2009, p. 75 (2P05), Tatranské Matliare, Slovakia, 07-11 September 2009.
87. Kovanda F., Mašátová P., Jirátová K.: Preparation of Layered Double Hydroxides on Metal Supports. XIV International Clay Conference, Book of Abstracts, p. 454, Castellaneta Marina, Italy, 14-20 June 2009.
88. Kraleva E., Spojakina A.A., Saladino M.L., Caponetti E., Jirátová K.: Preparation of Mixed Titania-Zirconia Nanostructured Materials Using Different Methods. EuropaCat IX: "Catalysis for Sustainable World", Abstracts, p. 541 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
89. Krejčíková S., Matějová L., Matěj Z., Jirkovský J., Šolcová O.: Preparation and Characterization of Ti - Zr Oxidic Thin Layers. Zing Catalytic Reactions Conference 2009, Poster Abstracts, p. 20, Antigua and Barbuda, 04-07 March 2009.
90. Krejčíková S., Matějová L., Šolcová O.: Příprava nanočástic kovových oxidů vhodných pro tenké vrstvy. (Czech) Preparation of the Nanoporous Doped Titania Layers. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 34 (4 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
91. Krejčíková S., Matějová L., Šolcová O., Čapek L.: Titania Nanofilms and Their Doped Equivalents. 3rd International Symposium Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 61, Albena, Bulgaria, 06-09 September 2009.
92. Krejčíková S., Matějová L., Šolcová O., Morozová M., Čapek L.: Doped Titania Layers for Photocatalysis. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 70 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
93. Kubička D., Horáček J., Kaluža L.: Tuning the Selectivity in Deoxygenation of Triglycerides Aimed at the production of Renewable Feedstocks for Ethylene Production. EuropaCat IX: "Catalysis for Sustainable World", Abstracts p. 424 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
94. Matějová L., Cajthaml T., Benada O., Matěj Z., Klusoň P., Šolcová O.: Extraction Techniques for Preparation of Well-Defined Photoactive Oxide Materials. Catalytic Reactions Conference 2009, Poster Abstracts, p. 8, Antigua and Barbuda, 04-07 March 2009.
95. Matějová L., Součková H., Cajthaml T., Šolcová O.: Extraction Techniques for Preparation of Metal Oxides. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 69 (4 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
96. Morozová M., Klusoň P., Krýsa J., Šolcová O.: Fotoelektrokatalytické procesy na tenkých vrstvách TiO_2. (Czech) Photoelectrocatalytic Processes on Thin TiO_2 Layers. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 221 (3 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
97. Morozová M., Klusoň P., Krýsa J., Šolcová O.: The Photoelectrocatalytic Properties of Thin TiO_2 Electode. 3rd International Symposium, Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 138, Albena, Bulgaria, 06-09 September 2009.

98. Morozová M., Klusoň P., Krýsa J., Zlámal M., Šolcová O.: Electrochemical Properties of Thin TiO_2 Layers. Catalytic Reactions Conference 2009, Poster Abstracts, p. 21, Antigua and Barbuda, 04-07 March 2009.
99. Morozová M., Klusoň P., Krýsa J., Zlámal M., Šolcová O.: Photoelectrochemistry on Thin TiO_2 Layers. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 48 (3 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
100. Obalová L., Karásková K., Jirátová K., Kovanda F.: Effect of Alkali Promoter Doping in Calcined Co-Mn-Al Layered Double Hydroxide on Catalytic Decomposition of N_2O. EuropaCat IX: "Catalysis for Sustainable World", Abstracts, p. 386 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
101. Palcheva R., Spojakina A.A., Dimitrov L., Jirátová K.: 12-Tungstophosphoric Heteropolyacid Supported on Modified SBA-15 as Catalyst in HDS of Thiophene. EuropaCat IX: "Catalysis for Sustainable World", Abstracts, p. 239 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
102. Petráš D., Soukup K., Klusoň P., Šolcová O.: Nanofiber Membranes ─ Evaluation of Transport Properties. 9th International Conference on Catalysis in Membrane Reactors, Book of Abstracts, pp. 227-228, Lyon, France, 28 June - 02 July 2009.
103. Ponec R.: Peculiarities of Metal-Metal Bonding. Insights from the Analysis of Domain Averaged Fermi holes. 3rd Japan-Czech-Slovak Symposium on Theoretical and Computational Chemistry, Proceedings, p. 25 (O-10), Bratislava, Slovakia, 09-12 September 2009.
104. Ponec R.: Chemical Structures from the Analysis of Domain Averaged Fermi holes. Peculiarity of Metal-Metal Bonding. International Symposium Molecular Informatics and Bioinformatics 2009, Collection of Abstracts, pp. 21-22, Budapest, Hungary, 17-19 March 2009.
105. Ponec R., Cooper D.L.: Anatomy of Bond Formation. Insights from the DAFH Analysis in Momentum Space. Central European Symposium on Theoretical Chemistry, Program, poster 33, Dobogókö, Hungary, 25-28 September 2009.
106. Ponec R., Feixas F.: Peculiarity of Cr-Cr Bonding. Insights from the Analysis of Domain Averaged Fermi holes. Workshop on Theoretical Chemistry 2009., Proceedings, p. 27, Platja d`Aro, Spain, 08-12 July 2009.
107. Setničková K., Jeřábek K., Uchytil P.: Pervaporace versus permeace par –rozdíly z hlediska transportu látek polymerní membránou. (Czech) Pervaporation vs. Vapor Permeation - Differences in Transport Properties of the Polymeric Membrane. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 44, Srní, Šumava, Czech Republic, 19-22 October 2009.
108. Soukup K., Rogut J., Ludwik-Pardala M., Wiatowski M., Šolcová O.: Hydrogen Storage by Redox Cycle of Iron/Iron Oxides. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 335 (4 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
109. Soukup K., Rogut J., Ludwik-Pardała M., Wiatowski M., Šolcová O.: Stanovení transportních charakteristik porézních pelet Fe2O3/Al2O3 využitelných pro uchovávání vodíku. (Czech) Determination of Transport Characteristics of Porous Pellets Fe2O3/Al2O3 Using for Hydrogen Storage. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 57 (5 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
110. Soukupová K., Sassi A., Jeřábek K.: Morphological Changes of Polystyrene Sorbents after Gamma-Rays Irradiation. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 234, Srní, Šumava, Czech Republic, 19-22 October 2009.
111. Svoboda K., Šolcová O., Pohořelý M., Hartman M.: Enhanced Coalbed Methane Recovery by Means of Carbon Dioxide. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 261 (15 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
112. Šolcová O., Maléterová Y., Matějová L., Kaštánek F.: Titania Catalysts for Advanced Oxidation Processes. Catalytic Reactions Conference 2009, Poster Abstracts, p. 9, Antigua and Barbuda, 04-07 March 2009.
113. Šolcová O., Matějová L., Šnajdaufová H., Schneider P.: Comparison of Nitrogen and Argon Physisorption for Precise Texture Characterization. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 71 (6 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
114. Topka P., Karban J., Soukup K., Šolcová O.: Evaluation on Textural, Mechanical, and Catalytic Properties of Al-SBA-15 Pellets with Low Content of Silica Binder. 41st Symposium on Catalysis, Program Book of Abstracts, pp. 76-77, Prague, Czech Republic, 02-03 November 2009.
115. Topka P., Soukup K., Karban J., Šolcová O.: Catalytic Activity of Al-SBA-15 Pellets with Low Content of Additives in Friedel-Crafts Alkylation. 3rd International Symposium Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 140, Albena, Bulgaria, 06-09 September 2009.

116. Topka P., Soukup K., Šolcová O.: Al-SBA-15 Pellets with Low Additive Content: Catalytic Activity in Friedel-Crafts Alkylation. EuropaCat IX: "Catalysis for Sustainable World", Abstracts, p. 568 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
117. Vít Z., Kaluža L., Gulková D., Zdražil M.: Effect of Pyridine on HDS of Thiophene over Ru and Rh Promoted Mo/Al_2O_3 Catalysts. EuropaCat IX: "Catalysis for a Sustainable World", Abstracts p. 329 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
118. Vít Z., Kaluža L., Gulková D., Zdražil M.: Inhibitive Effect of Pyridine on HDS over Mo/Al_2O_3 Modified by Noble Metals. 41st Symposium on Catalysis, Program Book of Abstracts, pp. 56-57, Prague, Czech Republic, 02-03 November 2009.
119. Vosecký M., Skoblia S., Jirátová K., Kameníková P., Pohořelý M., Punčochář M.: Identification of Carbon Deposits on the Nickel-Based Catalyst Used for the Steam Reforming of Biomass Tar at 500 °C. EuropaCatIX: "Catalysis for a Sustainable World", Abstracts p. 419 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
120. Žabová H., Církva V.: Preparation and Characterization of TiO_2 and Mn^+/TiO_2 and Their Utilization in Microwave Assisted Photocatalytic Reactions. 2nd China-Japan Symposium on Advanced Photocatalytic Materials (CJSAPM 2009), Program and Abstracts, pp. 54-55 (O-17), Nanjing, China, 05-07 March 2009.

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Fields of research

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

Research projects

Wall effect in flowing microdisperse liquids: apparent slip and electrokinetical potential
(O. Wein, joint project with TU 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 ED friction probes, including their automated calibration, has been extended to non-linear velocity profiles. AWS viscometry and routine measuring of zeta-potential have been applied for a class of nanofluids, prepared using several different dispersing methods. [Refs. 13-15, 27, 44, 50, 52]

Dynamics of bubble formation at submerged orifices: Simultaneous formation and synchronous regimes
(P. Stanovský, supported by ASCR, grant No. KJB200720901)

The goal of this project is an experimental study of the dynamics of interfacial meniscus inside an orifice during bubble formation from a submerged orifice. Incorporation of the meniscus dynamics into a mathematical model of the bubble formation allows explaining aperiodicity in the bubble formation at one orifice. The project objectives are the experimental verification of the model in a wide range of parameters coupled with the study of interactions between external acoustic source and the meniscus motion. Finally, an extension of the model from one orifice to more orifices will be 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. 34-36, 54]

Determination of the coalescence efficiency of bubbles in liquids
(S. Kordač Orvalho, supported by GACR, grant No. GP104/09/P255)

The coalescence phenomenon is of capital importance in the design and performance of multiphase contactors. Although studied for several decades, it is still not completely understood. The present project aims to improve our knowledge on the subject in the following way: to determine experimentally a relation between coalescence efficiency and the crucial control parameters (bubble properties, liquid properties, liquid flow conditions). Bubble coalescence will be studied experimentally in a laboratory cell (pairwise first, multiple then) under well-defined conditions. Then, these small scale data will be related to the coalescence in real gas-liquid dispersions in bubble column reactors. [Refs. 6, 33]

Analysis of hydrodynamic forces acting on bubbles by PIV measurements
(J. Vejražka, supported by ASCR, grant No. IAA200720801)

The liquid flow in proximity of bubbles is studied experimentally by using the time-resolved particle image velocimetry and high-speed flow visualizations. The measured velocity field will be treated in order to get information on the forces acting on bubbles in different flow situations. The calculation and analysis of the viscous dissipation and inertia of liquid in motion will be performed for various situations both in pure liquids and in surfactant solutions. The results will enlarge the knowledge of bubble flow dynamics, required to improve computational models used for the prediction of macroscopic two-phase flows. [Refs. 12, 16, 45-48, 54]

Hydrodynamics of bubble-particle interactions under liquid circulation
(M. Zedníková, supported by ASCR, grant No. KJB200720801)

The project deals with bubble-particle interactions under liquid circulation. Theoretical description exists only for small particle-large bubble interactions, used in mineral flotation. If the objects proportion is inverted, the mechanism of interaction is no longer fully understood. Thus, the objectives of the project are to study: i) small bubble-large particle interactions under liquid circulation and ii) interaction of more bubbles with a particle and formation of stable bubbles-particle aggregate. The bubble trajectory, velocity, momentum and deformation during impact are obtained by high speed camera visualization and the liquid velocity flow field is measured by PIV. The experimental data will create a base for theoretical description of bubble-particle interactions. [Refs. 16, 49, 53-56]

Transport and reaction processes in complex multiphase systems
(J. Drahoš, joint project with ICT and UPa, supported by GACR, grant No. GD104/08/H055)

Project is focused on training of doctoral students in the field of chemical engineering via targeted research in modern branches of chemical, pharmaceutical, biological and process industries with emphasis on research in new areas such as micro- and nanotechnologies and material engineering. It includes theoretical and experimental work of 20 students of Chemical Engineering Departments at ICT and UPa, and at ICPF. Particular research programmes involve 16 areas from microsystems to industry-scale processes. Project will be led by 18 supervisors. The training includes both general courses on mathematical modeling, statistical analysis and methodology of scientific work, and courses specialized on specific research fields. Students will take part in national and international projects of cooperation with major research laboratories. The project output will be publications in impacted international journals, presentations at conferences and special workshops with lectures by students, supervisors and invited specialists, published in proceedings. [Refs. 19-21, 26, 28-32]

Presidency of the European Federation of Chemical Engineering (EFCE)
(J. Drahoš, supported by MEYS, INGO project No. LA 319)

The EFCE is one of the most important institutions in the field of chemistry. Prof. Jiří Drahoš successfully served for two years as its President. In September 2007 he has been re-elected as the President for the period 2008-2009. Together with Prof. Růžička, he also participated at the activities of the EFCE Working Party Multiphase Fluid Flow.

Hydrodynamics and transport phenomena in multiphase systems: from microscale to macroscale
(M. Růžička, joint project with TU Ostrava, supported by GA CR, grant No. GA104/07/1110)

The 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) will be 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 will be 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. 7-9, 12, 16]

Hydrodynamic concept of stromatactis formation in geology
(M. Růžička, joint project with Institute of Geology of the ASCR, v. v. i., supported by ASCR, grant No. IAAX 00130702)

The 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 proposed interdisciplinary study is novel, and the results would be fundamental for sedimentology and hydrodynamics, with possible implications in related technologies. [Refs. 26, 28-30]

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

Experimental part of the project consists in studying fast transient processes driven by a step change of voltage in electrolytic microcells. In the first year of the project, an experimental set-up (electrolytic cells, working electrodes, measuring and controlling hardware) were prepared and tested. The programs for PC-driven process control and data acquisition, written under LabView, were prepared and tested. This preparatory activity is documented in a series of 3 research reports. The related results in electrodiffusion diagnostics of flow were published. [Refs. 13-15, 27, 41-43, 50-52]

International co-operations

CRTT, Saint Nazaire, France: Backward-facing step flows, Microfluidics
LEGI / IMG, Grenoble, France: Bubble columns, Optical probes
Institute of Fluid Mechanics, Toulouse, France: Hydrodynamic interactions of bubbles
Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow
University of Minho, Braga, Portugal: Multiphase bubble bed reactors
University of Porto, Porto, Portugal: Hydrodynamics of g-l-s systems
Institute of Chemical Engineering, BAS, Sofia, Bulgaria: Gas-liquid reactors
Institute of Thermophysics, RAS, Russia: Diagnostics of multiphase flows
Worchester Polytechnic Institute, Worchester, USA: CFD
Technology Institute, SINTEF, Trondheim, Norway: Bubble columns
Kyoto University, Japan: Hydrodynamics of bubbly flow
Kobe University, Japan: Hydrodynamics of bubbly flow

Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)
M. Zedníková: University of Nottingham, Great Britain (6 weeks)
M. Šimčík: University of Braga, Portugal (3 months)
P. Novák: University of Braga, Portugal (1 month)

Visitors

S. Sharaf, University of Nottingham, UK
N. Abi Chebel, LGC Toulouse, France
E. Berich, University of Nantes, France
E.Cachaza, University of Salamanca, Spain
T. Abadie, INP Toulouse, France
L. Saint-Lary, INP Toulouse, France
P. Gajowka, INP Toulouse, France
C. Nickel, INP Toulouse, France
S.D. Vlaev, BAS, Sofia, Bulgaria

Teaching

J. Drahoš: ICT, postgraduate course "Multiphase reactors"
M. Růžička: ICT, postgraduate courses "Multiphase reactors", "Multiphase hydrodynamics"
J. Tihon: ICT, postgraduate course "Drops, bubbles, and particles"
J. Havlica: UJEP, courses "Introduction to MATLAB" and "Mathematics"

Publications

Original papers

1. Gogová Z., Hanika J.: Reactivation of a Palladium Catalyst during Glucose Oxidation by Molecular Oxygen. Chem. Pap. 63(5), 520-526 (2009).
2. Gogová Z., Hanika J.: Dynamic Modelling of Glucose Oxidation with Palladium Catalyst Deactivation in Multifunctional CSTR; Benefits of Periodic Operation. Chem. Eng. J. 150(1), 223-230 (2009).
3. Gogová Z., Hanika J.: Model-Aided Design of Three-Phase Gas-Lift Reactor for Oxidation Accompanied by Catalyst Reversible Deactivation. Chem. Eng. Technol. 32(12), 1929-1940 (2009).
4. Jelínek K., Pavlů J., Havlica J., Wild J.: Experimental Test of the Evans' B(3)-Field: Measuring the Interaction with Free Electrons. Found. Phys. 39(10), 1191–1196 (2009).
5. Lehnert R., Novák Pavel, Macieira F., Kuřec M., Teixeira J.A., Bányik T.: Optimisation of Lab-Scale Continuous Alcohol-Free Beer Production. Czech J. Food Sci. 27(4), 267-275 (2009).
6. Orvalho S.P., Růžička M., Drahoš J.: Bubble Column with Electrolytes: Gas Holdup and Flow Regimes. Ind. Eng. Chem. Res. 48(18), 8237-8243 (2009).
7. Růžička M.: Dripping Faucet and Bubbling Faucet: An Analogy. Chem. Eng. Res. Des. 87(10), 1366–1370 (2009).
8. Růžička M., Bunganič R., Drahoš J.: Meniscus Dynamics in Bubble Formation. Part I: Experiment. Chem. Eng. Res. Des. 87(10), 1349–1356 (2009).
9. Růžička M., Bunganič R., Drahoš J.: Meniscus Dynamics in Bubble Formation. Part II: Model. Chem. Eng. Res. Des. 87(10), 1357-1365 (2009).
10. Veselý V., Hanika J., Drahoš J.: Petelýza, chemická recyklace PET lahví. (Czech) Petelysis, Chemical Recycling of PET Bottles. Waste Forum 26-29 (2009).
11. Tihon J., Pěnkavová V., Pantzali M.: The Effect of Inlet Pulsations on the Backward-Facing Step Flow. Eur. J. Mech. B-Fluids, in press.
12. Vejražka J., Večeř M., Orvalho S.P., Sechet P., Růžička M., Cartellier A.: Measurement Accuracy of a Monofiber Optical Probe in a Bubbly Flow. Int. J. Multiphase Flow, submitted.
13. Wein O.: Convective Diffusion from Strip-like Microprobes into Colloidal Suspensions. Int. J. Heat Mass Transfer, in press.
14. Wein O.: Convective Diffusion from Convex Microprobes into Colloidal Suspensions: The Edge Effects. . Int. J. Heat Mass Transfer, in press.
15. Wein O.: Autocalibration of Electrodiffusion Friction Probes in Microdispersion Liquids. Int. J. Heat Mass Transfer, in press.
16. Zedníková M., Vobecká L., Vejražka J.: Effect of Solid Material and Surfactant Presence on Interactions of Bubbles with Horizontal Solid Surface. Can. J. Chem. Eng., in press.

Chapters in books

17. Wichterle K., Růžička M.: Scale-up Fundamentals. In: Scale-up in Metallurgy, ProcessEng Engineering GmbH Publishing, Viena, in press.

Patents

18. Veselý V., Drahoš J., Šírek M.: Způsob chemické recyklace odpadního polyethylentereftelátu. (Czech) Waste PET Chemical Recycling. Pat. No. PV 2006-550/CZ 301118. Applied: 06.09.08, Patented: 09.10.02.

International conferences

19. Baszczyński M., Kuřec M., Novák Pavel, Bányik T., Růžička M., Drahoš J.: Assessment of Yeast Aging by Flow Cytometry. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 317 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
20. Baszczyński M., Novák Pavel, Bányik T., Zedníková M., Růžička M., Drahoš J.: Vliv surfaktantů na stabilitu pivní pěny. (Czech) Influence of Surfactant on Beer Foam Stability. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 181, Srní, Šumava, Czech Republic, 19-22 October 2009.
21. Baszczyński M., Novák Pavel, Zedníková M., Bányik T., Růžička M., Drahoš J.: Beer Foam as a Multi-Phase Flow System: A Case Study. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 58 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
22. Fialová M., Orvalho S.P., Zedníková M., Růžička M., Drahoš J.: Vliv koalescence na zádrž plynu a objemový koeficient přestupu hmoty v bublané koloně. (Czech) Effect of Coalescence on Gas Holdup and

Volumetric Mass Transfer Coefficient in Bubble Column. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 260, Srní, Šumava, Czech Republic, 19-22 October 2009.

23. Fialová M., Zedníková M., Tovčigrečko V., Růžička M., Drahoš J.: Application of the Dynamic Pressure Step Method for kLaL Measurement with Air and Pure Oxygen in Bubble Column. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 345, Tatranské Matliare, Slovakia, 25-29 May 2009.
24. Gogová Z., Hanika J.: Multifunctional Reactors for Oxidation Accompanied with Reversible Catalyst Deactivation. 8th World Congress of Chemical Engineering (WCCE8), Abstract Book, p. 1172 (6 pp. full text on CD-ROM), 1186, Montreal, Canada, 23-27 August 2009.
25. Gogová Z., Hanika J.: Composition Modulation of Catalytic Reactors. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 84 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
26. Hladil J., Kulaviak L., Růžička M.: Pattern Formation in Geological Sediments: Field Observation versus Experiments in a Glass of Water. 5th European-Japanese Two-Phase Flow Group Meeting, invited lecture, Spoleto, Italy, 20-25 September 2009.
27. Kantorová J., Večeř M., Wein O.: Vliv materiálu viskozimetrického senzoru na zdánlivý skluz při stěně. (Czech) Effect of the Viscometric Sensor's Material on Apparent Wall Slip. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 195, Srní, Šumava, Czech Republic, 19-22 October 2009.
28. Kulaviak L., Růžička M., Drahoš J., Hladil J.: Parameters Affecting Process of Particles Sedimentation. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 349, Tatranské Matliare, Slovakia, 25-29 May 2009
29. Kulaviak L., Růžička M., Drahoš J., Hladil J.: Spatial Distribution of Particles and Cavities in Sedimentary Deposits. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 1, Tatranské Matliare, Slovakia, 25-29 May 2009.
30. Kulaviak L., Růžička M., Drahoš J., Hladil J.: Parameters Affecting Process of Particles Sedimentation (2. Campaign). 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 193, Srní, Šumava, Czech Republic, 19-22 October 2009.
31. Novák Pavel, Baszczyński M., Bránýik T., Zedníková M., Růžička M., Drahoš J.: Sledování vlivu surfaktantů na tvorbu pivní pěny pomocí rychloběžné kamery. (Czech) High-speed Imaging of Beer Foam Formation: Effect of Surfactants. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 203, Srní, Šumava, Czech Republic, 19-22 October 2009.
32. Novák Pavel, Baszczyński M., Orvalho S.P., Bránýik T., Růžička M., Drahoš J.: Interaction of Gas Bubbles with Solid Particles in Continuous Beer Fermenting System with Potential for Foaming. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 60 (5 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
33. Orvalho S.P., Růžička M., Drahoš J.: Coalescence of Bubbles: A Case Study. 8th World Congress of Chemical Engineering, Abstract Book, p. 1247, Montréal, Quebec, Canada, 23-27 August 2009.
34. Stanovský P., Růžička M.: Uniformity of Bubble Formation at Submerged Orifices. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 346, Tatranské Matliare, Slovakia, 25-29 May 2009.
35. Stanovský P., Růžička M.: Vliv operačních parametrů na periodicitu tvorby bublin na otvoru. (Czech) Influence of the Operational Parameters on the Periodicity of Bubble Formation at the Orifice. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 258, Srní, Šumava, Czech Republic, 19-22 October 2009.
36. Stanovský P., Růžička M., Drahoš J., Sanada T., Shirota M, Sato A., Watanabe M.: Pairwise Interaction of Bubbles at Moderate Reynolds Numbers. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 256 (2pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
37. Šimčík M., Mota A., Havlica J., Růžička M., Vincente A., Teixeira J.: CFD Simulation of Residence Time Distribution in Airlift Reactor and Bubble Column. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 352, Tatranské Matliare, Slovakia, 25-29 May 2009.
38. Šimčík M., Růžička M., Drahoš J.: Calculation of Bubble Added Mass Using VOF Model. 8th World Congress of Chemical Engineering, Abstract Book, p. 1242, Montréal, Quebec, Canada, 23-27 August 2009.
39. Šimčík M., Růžička M., Drahoš J.: Estimation of Added Mass in Dispersion: CFD Approach. 5th European-Japanese Two-Phase Flow Group Meeting, invited lecture, Spoleto, Italy, 20-25 September 2009.

40. Tihon J., Pěnkavová V., Vejražka J.: Experiments on Large Bubbles Rising in an Inclined Flat Channel. 5th International Berlin Workshop on Transport Phenomena with Moving Boundaries, pp. 1-14, Berlin, Germany, 08-09 October 2009.
41. Tihon J., Pěnkavová V., Vejražka J.: Wall Shear Stress under Large Bubbles Rising in an Inclined Channel. Experimental Fluid Mechanics 2009, Proceedings, pp. 357-367, Liberec, Czech Republic, 25-27 November 2009.
42. Tihon J., Pěnkavová V., Vejražka J.: Experimentální studium pohybu bublin v nakloněném plochém kanálu. (Czech) Experiments on Large Bubbles Rising in an Inclined Flat Channel. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 257 (16 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
43. Tihon J., Pěnkavová V., Vejražka J.: Experiments on Large Bubbles Rising in an Inclined Flat Channel. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 338 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
44. Večeř M., Pěnkavová V., Langmaier J.: Viskozimetrie iontových kapalin. (Czech) Rheology of Ionic Liquids. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 190, Srní, Šumava, Czech Republic, 19-22 October 2009.
45. Vejražka J., Orvalho S., Vobecká L., Zedníková M., Tihon J.: Bubble Oscillations and Their Damping by Surfactants. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 350 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
46. Vejražka J., Orvalho S.P., Vobecká L., Zedníková M., Tihon J.: Tlumení tvarových oscilací bublin surfaktanty. (Czech) Damping of Bubble Shape Oscillations by Surfactants. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 259, Srní, Šumava, Czech Republic, 19-22 October 2009.
47. Vejražka J., Vobecká L., Fujasová-Zedníková M., Orvalho S.P., Tihon J.: Damping Time of Bubble Oscillations in Clean Liquids and in Surfactants. 5th International Berlin Workshop on Transport Phenomena with Moving Boundaries, pp. 1-14, Berlin, Germany, 08-09 October 2009.
48. Vejražka J., Vobecká L., Zedníková M., Orvalho S.P., Tihon J.: Effect of Surface Viscoelastic Properties on Bubble Oscillations. Experimental Fluid Mechanics 2009, Proceedings, pp. 376-388, Liberc, Czech Republic, 25-27 November 2009.
49. Vobecká L., Zedníková M., Vejražka J., Růžička M.: Studium interakcí bubliny s pevným povrchem, vliv koncentrace surfaktantu a druhu povrchu. (Czech) The Study of Interactions of Bubbles with Solid Surface. The Effect of Surfactant Concentration and Type of Solid Surface. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 137 (7 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
50. Wein O., Tovčigrečko V., Sobolík V., Večeř M.: Diagnostics of Apparent Wall Slip in Aqueous Polymer Solutions. Novel Trends in Rheology III, Proceedings , pp. 139-151, Zlín, Czech Republic, 28-29 July 2009.
51. Wein O., Tovčigrečko V., Večeř M., Sobolík V.: Electrodiffusion Diagnostics of Apparent Wall Slip in Polymer Solutions. 5th Annual European Rheology Conference, Scientific Programme and Abstracts, p. 1, Cardiff, Wales, Great Britain, 15-17 April 2009.
52. Wein O., Tovčigrečko V., Večeř M., Sobolík V.: Electrodiffusion Diagnostics of Apparent Wall Slip in Polymer Solutions. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 141 (16 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
53. Zedníková M., Růžička M., Drahoš J.: Výzkum vícefázových systémů na ÚCHP AV ČR Praha. (Czech) Research of Multiphase Systems at ICPF AS CR Prague. 8. Mezinárodní konference a výstava ODPADNÍ VODY – WASTEWATER 2009, Konferenční sborník, pp. 303-308 (full text on CD-ROM), Plzeň, Czech Republic, 05-07 May 2009.
54. Zedníková M., Vejražka J., Vobecká L., Růžička M.: Effect of Surfactant on a Bubble Bouncing on a Wall. 8th World Congress of Chemical Engineering, Abstract Book, p. 472, Montréal, Quebec, Canada, 23-27 August 2009.
55. Zedníková M., Vobecká L., Vejražka J., Růžička M., Drahoš J.: Effect of Liquid and Solid Properties on Bubble-Wall Collisions. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 343 (8 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
56. Zedníková M., Vobecká L., Vejražka J., Růžička M.: Kolize bubliny s částicí v proudu kapaliny. (Czech) Bubble-Particle Collision in Liquid Circulation. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 254, Srní, Šumava, Czech Republic, 19-22 October 2009.

Department of New Processes in Chemistry and Biotechnology

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Fields of research

- Bioremediation of organic pollutants in soil and sewage
- Immobilization of biocatalysts, living cells or enzymes, into organic or organic-inorganic matrices by sol-gel process
- Application of immobilized biocatalysts in optical sensors
- Polymeric antidegradants immobilized on poly(siloxanes)
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphase media
- Carbosilane dendrimers

Applied research

- Complex dehalogenation of PCB contaminated soils, waste water and oils

Research projects

The research and verification of the method of catalytic dehalogenation of underground water from industrial sources by bimetallic permeable barriers
(F. Kaštánek, supported by MIT, IMPULS project No. FI-IM3/050)

The response rate of the reductive dehalogenation of halogenated (aliphatic chlorinated hydrocarbons) and polyhalogenated organic compounds (PCB) was studied. The efficiency was tested in the real decontamination process of water contaminated by polychlorinated ethanes and ethylenes. The pilot test was successfully accomplished in the chemical factory Spolana Neratovice during the experiments of cleaning-up of the underground water contaminated by chlorinated alkanes (bimetallic barrier was composed of the layer of the grey graphite iron + 0.3% of Pd – results were published in the final Report of the project (in Czech). [Refs. 9, 10, 20, 23]

Enhancement of the economy of biogas units
(F. Kaštánek, supported by ČEZ 2009.S079.02)

The aim of project was the experimental verification of a proposed novel technology of energy and materials production, consisting of the following steps: production of biogas from agricultural wastes, presumed utilization of biogas for electricity and heat production in association with the use as a source of carbon dioxide for microalgae cultivation. The microalgal biomass can be hereafter processed to valuable products such as food and feed supplements. A part of the process wastewater can be utilized as a nitrogen source for microalgae cultivation, so the whole process is technologically closed. The tests were performed in a pilot–scale photobioreactor (volume 300 L). [Refs. 11, 21]

The structure and synthetic applications of transition metal complexes
(J. Čermák, joint project with JH IPC, CU, and ICT, supported by MYES, project No. LC06070)

Synthesis of helicenes starting from 1,8-diarylnaphthalenes was attempted and a mechanism of byproduct formation proposed. Peripheral substitution of carbosilane dendrimers by cyclopentadienes and cyclopentadienyl complexes afforded immobilized dichlorotitanocenes, potential catalysts for alkene hydrogenation. Their efficient purification was achieved with the aid of preparative GPC. A novel type of heavy fluorous cyclopentadienes bearing three or six polyfluoroalkyl chains was synthesized and their first titanium complexes were prepared and characterized. Dynamics of metallotropic shifts in these silyl-substituted cyclopentadienes was studied by variable temperature NMR. [Refs. 2, 3, 6, 7, 13, 17, 18, 24, 27]

Interaction of organic-inorganic matrices with immobilized biological material
(G. Kuncová, supported by the MEYS, OC COST project No. OC121)

Novel organic-inorganic hybrid composites containing porphyrins producing singlet oxygen were prepared and characterized by porosimetry, scanning electron microscopy, fluorescence and diffuse reflectance UV-VIS spectroscopy. It was found that porphyrins are immobilized in the poly(hydroxymethylsiloxane) matrix in the free-base monomer form. Their irradiation produced singlet oxygen $O_2(^1\Delta_g)$ with the lifetime of 10–30 μs. [Refs. 1, 5, 11, 12, 14-16]

Polymeric antidegradants based on liquid polybutadienes, polysiloxanes and their block copolymers
(J. Hetflejš, joint project with IMC, SYNPO Pardubice, and UPa, supported by GA CR, grant No. GA203/07/0987)

Low molecular OH-ended antidegradants based on sterically hindered piperidine (HALS) attached to a short siloxane chain have been prepared in high yields and purity using novel protocols. The compounds were efficient polyurethane stabilizers acting simultaneously as molecular-weight regulators. [Refs. 4, 8]

Monitoring and remediation of environmental pollution with advanced organic-inorganic materials – MOREPIM
(G. Kuncová, supported by MEYS, KONTAKT project No. ME 892)

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

Whole cell optical sensors (WOCOS)
(G. Kuncová, supported by MEYS, KONTAKT project No. ME 893)

Bioluminescent bioreporter *Pseudomonas putida TVA8* was tested as selective whole-cell biosensor of BTEX (benzene, toluene, xylene and ethylbenzene). We attempted to induce bioluminescence in this strain with 23 compounds to better discriminate response selectivity. The repeatable sensors were prepared by encapsulation of cells into silica based matrices. The cells were encapsulated both in thick layers and on the tips of optical fibres to prepare biosensors in remote localities. The biosensor applicability was demonstrated by comparison of its bioluminescence response towards exposition to influent and effluent of the waste water treatment of the chemical factory in the Czech Republic. [Refs. 25, 26]

Enzymatically catalyzed synthesis of alkyd resins (ENZALKYD)
(G. Kuncová, joint project with SYNPO Pardubice, supported by MIT, project No. MPO 2A-3TP1/108)

The research has been focused on enzymatic glycerolysis of soybean oil with aim to prepare optimal composition of a precursor for synthesis of special alkyd resins.

Optical chemical sensors - OPTISENS
(G. Kuncová, joint project with University of Maribor, Slovenia, supported by MEYS, KONTAKT project No. MEB 090817)

Novel recognition elements of pH sensors suitable for evaluation of yeast acidification power were prepared by absorption or entrapment of pH sensitive sulfonphthalein dyes into hydrogel of poly(2-hydroxyethyl methacrylate-co-ethylene dimethacrylate), or into co-polymer of tetramethoxysilane with 3-glycidoxypropyltrimethoxysilane (GPTMS). The pH sensitive films were characterized by pK_a values, response times, reversibility, and leaching of the dyes, and further evaluated with regard to its application in food industry. [Refs. 25, 26]

Novel inorganic-organic hybrid nanomaterials
(S. Šabata, joint project with ICT Praha, IMC, University of West Bohemia Plzeň, supported by ASCR, grant No. IAAX08240901)

The aim of project is preparation, characterization, and study of properties of inorganic/organic hybrid materials based on montmorillonite and calixarenes. Intercalated structures will be synthesized from various homoionic forms of the mineral using different synthetic methods depending on calixarene used. Special attention will be paid to metal complexation, both in the course of the introduction of organic guest into montmorillonite containing already metal cations in the interlayer spacing, and during intercalation of basic montmorillonite host by different calixarenes that can serve as ionofors. Derivatization of calixarenes by organosilicon moieties will enable the formation of siloxane bonding between host and guest molecules leading to stable hybrid nanomaterials with covalently bonded calixarenes. Hybrid structures will be studied for their potential application in catalytic reactions, neutral compounds recognition/intercalation, and their use for immobilization of enzymes. [Ref. 19]

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

Recently described attractive interactions between fullerene and porphyrin moieties will be used for the construction of receptors for selective complexation of fullerenes. Using the chemistry of calixarenes and/or thiacalixarenes novel well-preorganized systems bearing two or more porphyrin units in mutually coplanar arrangement will be prepared. These

compounds should enable synchronous cooperative interactions of porphyrins with fullerenes to form the sandwich type of complexes, thus operating as the molecular tweezers. Our preliminary experiments indicated that this type of receptors leads to strong complexation of fullerenes with surprisingly high selectivity towards fullerene C70. Potential selective complexation of higher fullerenes will be studied within this project, too. Immobilization of molecular tweezers on silica gel using sol-gel methodology could give novel materials suitable for the purification of crude fullerite soot. The results of this project could yield novel selective complexation agents enabling the construction of novel materials useful in the isolation, purification and analysis of fullerite soot, and hence to the reduction of the manufacturing expenses of fullerenes.

International co-operations

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

Center for Environmental Biotechnology University of Tennessee, 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

Teaching

F. Kaštánek: ICT, course "Bioengineering"

J. Čermák: UJEP, courses "Organic chemistry I" and "Organic chemistry II"

Publications

Original papers

1. Kuřec M., Kuncová G., Brányik T.: Yeast Vitality Determination Based on Intracellular NAD(P)H Fluorescence Measurement during Aerobic-Anaerobic Transition. Folia Microbiol. 54(1), 25-29 (2009).
2. Pošta M., Čermák Jan, Vojtíšek P., Sýkora J., Císařová I.: Diphosphinoazine Rhodium(III) and Iridium(III) Octahedral Complexes. Inorg. Chim. Acta 362(1), 208-216 (2009).
3. Storch J., Sýkora J., Čermák Jan, Karban J., Císařová I., Růžička A.: Synthesis of Hexahelicene and 1-Methoxyhexahelicene via Cycloisomerization of Biphenylyl-Naphthalene Derivatives. J. Org. Chem. 74(8), 3090-3093 (2009).
4. Šabata S., Blechta V., Karban J., Pleska A., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. Polish J. Chem. 83(11), 1953–1958 (2009).
5. Šabata S., Hetflejš J., Rychtáriková R., Kuncová G., Lang K., Kubát P.: Immobilization of Porphyrins in Poly(hydroxymethylsiloxane). Chem. Pap. 63(4), 438-444 (2009).
6. Čermák Jan, Krupková A., Auerová K., Zamrzla M., Nguyen Thi T.H., Vojtíšek P., Císařová I.: Tetramethyl(perfluoroalkyl)cyclopentadienyl Rhodium(I) Complexes with Ethylene or Diene Ligands. Crystal Structure of [(eta-5-$C_5Me_4C_6F_{13}$)Rh$(CO)_2$]. J. Organomet. Chem., in press.
7. Červenková Šťastná L., Čermák Jan, Cuřínová P., Sýkora J.: Synthesis and Fluxional Behavior of New "Haevy Fluorous" Cyclopentadienes. J. Organomet. Chem., in press.
8. Hetflejš J., Šabata S., Podešva J., Kovářová J., Prokůpek L., Netopilík M., Spěváček J., Sýkora J.: Novel Stabilizers Acting Simultaneously as Molecular-Weight Regulators of Soluble Elastomeric Polyurethanes. Polym. Degrad. Stabil., in press.

9. Kaštánek F., Kaštánek P., Maléterová Y.: Dechlorination of PCBs in Aqueous Mixtures with Zero-Valent Iron in Statu Nascendi. Influence of Microwaves on the Rate of Reaction. J. Hazard. Mater., submitted.
10. Kaštánek P., Kaštánek F., Hájek M.: Microwave-enhanced Thermal Adsorption of Polyhalogenated Biphenyls from Contaminated Soil. J. Hazard. Mater., submitted.

Review papers

11. Rychtáriková R., Kuncová G.: Imobilizované fotosenzitizátory singletového kyslíku a jejich účinek na mikroorganismy. (Czech) Immobilized Singlet Oxygen Photosensitizers and Their Antimicrobial Effect. Chem. Listy 103(10), 800-813 (2009).

Chapters in books

12. Kuncová G., Trögl J.: Physiology of Microorganisms Immobilized into Inorganic Polymers. In: Inorganic Polymers: Development, Properties, and Applications, Nova Science Publishers, New York, in press.

Patents

13. Storch J., Čermák Jan: Způsob přípravy racemických substituovaných helicenů. (Czech) Preparation of Racemic Substituted [6]Helicenes. Pat. No. PV 2008-831/CZ 301384. Applied: 08.12.22, Patented: 09.12.30.

International conferences

14. Bolyó J., Mair T., Kuncová G.: The Metabolic Synchronization of Immobilized Yeast Cells: Effect of Matrices. Conference on Functional Dynamics, Book of Abstracts, 2 pp., Cascais, Portugal, 02-05 March 2009.
15. Bolyó J., Mair T., Kuncová G., Hauser M.J.B.: Metabolic Synchronization of Encapsulated Yeast Cells: Effect of Gel Matrices. XVIIth International Conference on Bioencapsulation, Book of Abstracts, pp.224-225(P65 1-4), Groningen, Netherlands, 24-26 September 2009.
16. Bolyó J., Mair T., Kuncová G., Hauser M.J.B.: Metabolic Synchronization of Encapsulated Yeast Cells: Effect of Gel Matrices. International Conference Applied Natural Sciences 2009, Book of Abstracts, p. 64, Trnava, Slovakia, 07-09 October 2009.
17. Čermák Jan, Žádný J., Vojtíšek P., Císařová I.: Diphosphinoazine Nickel Complexes: Surprising Reactivity. XVIII EuCheMS International Conference on Organometallic Chemistry, Book of Abstracts, p. P-20, Gothenburg, Sweden, 22-25 June 2009.
18. Červenková Šťastná L., Čermák Jan: Fluorinated Silylcyclopentadienes and Their Titanium(IV) Complexes. 19th International Symposium on Fluorine Chemistry, Book of Abstracts, p. 174, Jackson Hole, USA, 23-28 August 2009.
19. Duchek P., Šabata S., Křenek T.: The Influence of Organic Modifier in a Commercially Available Organoclay on the Intercalation Process. International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2009, p. 344 (D-240), Guwahati, India, 09-11 December 2009.
20. Jandová J., Kaštánek F., Vu H.N., Štěpánek R., Maléterová Y., Šolcová O.: Comparison of Efficiency of Catalytic Reductive Dehalogenation of Polyhalogenated Compounds (PCBs, PBDE) in Aqueous Solutions with Selected Bimetallic Catalysts: Fe/Pd, Zn/Pd, Ni/Pd, Al/Pd, Mg/Pd. Catalytic Reactions Conference 2009, Poster Abstracts, p. 8, Antigua and Barbuda, 04-07 March 2009.
21. Kaštánek F., Braniyková I., Maléterová Y., Kaštánek P.: Využití destilačního odpadu v sekvenci bioplyn-kogenerace-produkce řas. (Czech) Utilization of Distillery Effluents and Agriculture Waste in a Biomas-Cogeneration-Microalgae Sequence. Seminář Biopaliva v dopravě, Book of Abstracts, 9 pp. full text on CD-ROM, Bratislava, Slovakia, 21-22 September 2009.
22. Kaštánek F., Maléterová Y., Šolcová O.: Catalytic Destruction of PCBs Dissolved in Aqueous and Oily Solutions. Influence of Microwaves on the Rate of Reaction. Catalytic Reactions Conference 2009, Poster Abstracts, p. 17, Antigua and Barbuda, 04-07 March 2009.
23. Kaštánek P., Kaštánek F., Hájek M., Sobek J., Šolcová O.: Dechlorination of Polychlorinated Biphenyl (PCB) in Contaminated Soils and Oils. 11th International Conference on Environmental Science and Technology - CEST 2009, Volume of Abstracts, p. 76, Chania, Kréta, Greece, 03-05 September 2009.
24. Krupková A., Čermák Jan, Walterová Z., Horský J.: Immobilization of Cyclopentadienyl Titanium(IV) Complexes on the Periphery of Carbosilane Dendrimers. 6th International Dendrimer Symposium 2009, Book of Abstracts, P1.27, Stockholm, Sweden, 14-18 June 2009.

25. Kuncová G., Pazlarová J., Adamová N., Hlavatá A., Ripp S., Sayler G.S.: Bioluminiscent Biosensor of Toluene. XVIIth International Conference on Bioencapsulation, Book of Abstracts, pp. 226-227(P66 1-4), Groningen, Netherlands, 24-26 September 2009.
26. Kuncová G., Trögl J., Gavlasová P., Ripp S.A., Sayler G.S.: The Influence of Immobilization into Silica Matrix on Response of Optical Whole-Cell Biosensors. 1st International Conference on Multifunctional, Hybrid and Nanomaterials, Delegate Manual, p. C1.2.09, Tours, France, 15-19 March 2009.
27. Sýkora J., Storch J.: LC-NMR in Organic Synthesis of Hexahelicene Derivatives. Magnetic Moments in Central Europe, Program and Book of Abstracts, p. 93, Otočec, Slovenia, 11-15 February 2009.
28. Šolcová O., Maléterová Y., Matějová L., Kaštánek F.: Titania Catalysts for Advanced Oxidation Processes. Catalytic Reactions Conference 2009, Poster Abstracts, p. 9, Antigua and Barbuda, 04-07 March 2009.
29. Vrbová H., Kuncová G., Pospíšilová M.: Optical Fiber Elements for Increasing Bioluminescence Coupling. 8. Česko-slovenská konference Trendy v Biomedicínskom Inžinierstve, Proceedings , pp. 229-233, Bratislava, Slovakia, 16-18 September 2009.

Environmental Process Engineering Laboratory

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Fields of research

- Persistent organic pollutants
- Fluidized bed combustion and gasification
- Gas-solid reactors and operations
- Gaseous and particulate emissions from combustion and industrial processes
- Solid waste treatment and co-combustion
- Preparation of the electrodeless discharge lamps for photochemical applications
- Investigation on the formation possibility of PCDD/F by synthetic reactions
- Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis

Applied research

- Dechlorination of persistent organic pollutants
- Recovery of precious metals
- PET recycling
- Electronic scrap recycling
- Microwave technology for waste recycling
- Low-energy microwave depolymerization of waste poly(ethylene terephthalate) (PET) and polyurethane (PUR) foams

Research projects

Near zero emission advanced fluidized bed gasification (FLEXGAS)
(M. Punčochář, supported by Research Fund for Coal and Steel (RFCS), project No. RFCR-CT-2007-00005)

In this project, the ways are examined of overcoming the potential disadvantages of fluidized bed gasification, the technology for CO_2 capture/reduction and the advantages in

terms of their ability to process biomass/waste in association with coal at different scales of operation and for different applications. [Refs. 4, 17, 20, 21, 37, 38, 42-44]

Phytoextraction biomass disposal – an unsolved problem

(M. Punčochář, joint project with Czech University of Life Sciences, supported by GA CR, grant No. GA104/07/0977)

Potentially toxic elements such as Cd or Zn accumulated in the biomass of hyperaccumulating and/or highly accumulating plants are bound into different parts of the organic matrix in different extent and direct extraction of these elements is not straightforward. The aim of the project is to grow different plant species with the ability to accumulate metals in above ground biomass mainly willows and to develop procedure degrading organic matrix of the element accumulating plants, into the forms, where elements could be effectively extracted and recovered. [Refs. 19, 40, 46, 48]

Waste as raw material and energy source

(M. Punčochář, joint project with Brno University of Technology, and EVECO Brno, 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. The project involves both experiments and computer simulations. [Refs. 18, 28, 51-53]

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

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

A fundamental understanding of such viable reaction systems for the thermal oxidation of organic liquids entrapped (absorbed) within porous solids is still lacking. The hydrodynamic behavior of the "g"-"s" suspensions with such polluted (wet and sticky) particles is explored with the aid of pressure fluctuations also with respect to their unwanted tendency to stick together and lie down. Hitherto unexplored, inert and porous particles soaked in model organic compounds will be fired in a bench-scale, fluid-bed reactor operated in different regimes. Experimental and modeling efforts seek to explain and describe the dependence of the reactor's combustion efficiency as a function of residence time, excess air, operating temperature and particle size. The study focuses on the overall picture of formation and oxidation destruction of main gaseous pollutants (NO, NO_2, N_2O, CO, organic residuals, persistent organic pollutants, SO_2, and HCl) and their interrelationships. [Refs. 1, 12, 13, 34]

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

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

Project is focused on gasification of waste biomass which comes from the production of bio-ethanol and bio-diesel. The aim is to produce hydrogen from biomass, to capture CO_2 rising in the process and to separate present heteroatoms. A specific task of the project is to develop the integral process which includes the processing of biomass into existing technology of waste crude oil gasification. [Refs. 5, 32, 33, 49]

PETELYSE-PET recycling

(V. Veselý, joint project with ICT, supported by MIT, IMPULS project No. FI-IM4/096)

The technology of PET recycling developed in ICPF consists in PET flakes crystallization. Formed crystalline PET is crushed into small particles and then is subject to the basic hydrolysis at atmospheric pressure. In addition to lye solution, glycol is added in the hydrolysis. Water is eliminated by boiling, which gives rise to suspension of sodium salt of terephthalic acid and glycol. The suspension is skimmed and the filtered glycol is vacuum distilled. Pure glycol is then the distillation product. Electrolysis removes pure terephthalic acid salt from the solution. Glycol solution is returned to the hydrolysis. Terephthalic acid is precipitated by a mineral acid. Terephthalic acid and glycol are products in a "polymer grade" quality. The waste is a part of washing waters, distillation remainders after glycol regeneration and a filter cake after the terephthalate solution filtration. The main aim of the project is to produce reliable data for scaling up of the process and to evaluate the economy of whole recycling. [Refs. 6, 25, 26, 29, 50]

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

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

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

Preparation of the electrodeless discharge lamps for photochemical applications

(V. Církva, supported by GA CR, grant No. GA104/07/0992)

The project is concerning on preparation of the electrodeless discharge lamps (EDLs) as a suitable source of UV/VIS light for photochemical reactions. The EDL consists of a glass tube filled under a lower pressure with an inert gas and an excitable substance (mercury, sulfur), and generates UV/vis radiation when placed into the microwave field. The effect of operating EDL parameters, the microwave power output and medium properties on spectral characteristics are studied. [Refs. 2, 7-11, 16, 22, 54]

Investigation on the formation possibility of PCDD/F by synthetic reactions from their surrogates

(V. Církva, supported by GA CR, grant No. GA104/07/1212)

The project is directed toward a study of the synthetic reactions producing persistent organic pollutants of the type of PCDD and PCDF, with special emphasis on the conditions of formation of these substances in combustion plants. Investigation is focused on the formation possibility of PCDD/F from their surrogates. As the major proposed surrogates are chlorinated phenols and benzenes. The research is also oriented on the formation study of new PCDD/F intermediates and precursors on suitable solid supports from corresponding surrogates. Attention is paid to the effects of matrices and of copper metal forms with various physico-chemical properties on the course of the synthetic reactions. The research results should contribute to initiation of further technical measures in combustion plants that would decrease PCDD/F emissions. [Refs. 3, 7, 8, 11, 54]

Immobilization of heavy metals in municipal waste incinerator materials

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

The combustion of municipal waste is one of ways to meet nowadays the EU requirements to reduction of amount of dumped waste. The municipal solid waste incinerators (MSWI) convert waste to energy and certain amount of solid waste materials – fly ash and

bottom ash. These solid residuals contain, besides other components, toxic heavy metals which have to be stabilized against leaching out from the waste material before it can be safely stored at a landfill. The MSWI solid waste materials have latent hydraulic or puzzolanic properties. This fact offers an effective way of heavy metals immobilization which will be studied in the present project.

Simultaneous cooling at microwave heating - a new method in heterogeneous catalysis
(M. Hájek, supported by GA CR, grant No. GA104/08/0416)

The research has been focused on application in heterogeneously catalyzed reactions in liquid phase. It has been observed that selectivity of catalytic reaction can be significantly improved. These important findings evoked continuation to study this effect in more detail, what is the subject of this project. Scope and limitation of this method including possibility of potential applications has been studied on model reactions with non-polar (non-absorbing) reactants (alkylation of aromatics by alkenes) in the presence of strong acidic (strong absorbing) solid catalysts. [Refs. 8, 10, 14, 39, 41, 47]

Low-energy microwave depolymerization of waste poly(ethylene terephthalate) (PET) and polyurethane (PUR) foams
(M. Hájek, J. Sobek, supported by ICPF)

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

Emission factors of POPs and heavy metals from small sources
(V. Pekárek, joint project with TU Ostrava, supported by MEYS, project No. SP/1a2/116/07)

Determination of emission factor for selected POPs compounds and heavy metals is solved. The following topics will be studied (i) the validation of the original air dilution unit for the sampling, (ii) effect of different combustion units from the standpoint of toxic compound emission, (iii) effect of different fuels on the toxic compounds formation. [Refs. 23, 35, 36, 45]

International co-operations

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

Teaching

M. Punčochář, P. Kameníková, M. Pohořelý and M. Vosecký: Czech University of Life Sciences Prague, course "Renewable and alternative sources of energy"

Publications

Original papers

1. Hartman M., Trnka O., Svoboda K.: Use of Pressure Fluctuations to Determine Online the Regime of Gas-Solids Suspensions from Incipient Fluidization to Transport. Ind. Eng. Chem. Res. 48(14), 6830-6835 (2009).
2. Kment Š., Klusoň P., Žabová H., Churpita A., Chichina M., Čada M., Gregora I., Krýsa J., Hubička Z.: Atmospheric Pressure Barrier Torch Discharge and its Optimization for Flexible Deposition of TiO_2 Thin Coatings on Various Surfaces. Surf. Coat. Technol. 204(5), 667-675 (2009).
3. Kuča K., Musilová L., Paleček J., Církva V., Paar M., Musílek K., Hrabinová M., Pohanka M., Zdarová Karasová J., Jun D.: Novel Bisquaternary Oximes — Reactivation of Acetylcholinesterase and Butyrylcholinesterase Inhibited by Paraoxon. Molecules 14(12), 4915-4921 (2009).
4. Svoboda K., Kalisz S., Miccio F., Wieczorek K., Pohořelý M.: Simplified Modeling of Circulating Flow of Solids between a Fluidized Bed and a Vertical Pneumatic Transport Tube Reactor Connected by Orifices. Powder Technol. 192(1), 65-73 (2009).
5. Tukač V., Hanika J., Veselý V., Lederer J., Nečesaný F.: Možnosti produkce vodíku parciální oxidací odpadní biomasy. (Czech) Possibility of Hydrogen Production by Partial Oxidation of Waste Biomass. CHEMagazín 19(3), 8-9 (2009).
6. Veselý V., Hanika J., Drahoš J.: Petelýza, chemická recyklace PET lahví. (Czech) Petelysis, Chemical Recycling of PET Bottles. Waste Forum 26-29 (2009).
7. Žabová H., Církva V.: Microwave Photocatalysis III. Transition Metal Ion-Doped TiO_2 Thin Films on Mercury Electrodeless Discharge Lamps: Preparation, Characterization and Their Effect on the Photocatalytic Degradation of Mono-Chloroacetic Acid and Rhodamine B. J. Chem. Technol. Biotechnol. 84(11), 1624-1630 (2009).
8. Žabová H., Církva V., Hájek M.: Microwave Photocatalysis II: Novel Continuous-Flow Microwave Photocatalytic Experimental Set-up with Titania-Coated Mercury Electrodeless Discharge Lamps. J. Chem. Technol. Biotechnol. 84(8), 1125-1129 (2009).
9. Žabová H., Dvořák B.: Gas Phase Degradation of Acetone Using a TiO_2 Photocatalyst Supported on a Polyester Fabric. Reac. Kinet. Catal. Lett. 98(1), 165-175 (2009).
10. Žabová H., Sobek J., Církva V., Šolcová O., Kment Š., Hájek M.: Efficient Preparation of Nanocrystalline Anatase TiO_2 and V/TiO_2 Thin Layers Using Microwave Drying and/or Microwave Calcination Technique. J. Solid. State Chem. 182(12), 3387-3392 (2009).
11. Církva V., Relich S., Hájek M.: Microwave Photochemistry V: Low-Pressure Batch and Continuous-Flow Microwave Photoreactors with Quartz Mercury Electrodeless Discharge Lamps. Photohydrolysis of Mono-Chloroacetic Acid. J. Chem. Technol. Biotechnol. 85(2), 185-191 (2010).
12. Hartman M., Trnka O., Pohořelý M.: Nové explicitní vztahy pro vyjádření termálních pádových rychlostí tuhých částic. (Czech) Novel Explicit Formulae to Estimate the Free-Fall Conditions for Solid Particles. Chem. Listy, in press.
13. Hartman M., Trnka O., Pohořelý M., Svoboda K.: High-Temperature Reaction in the Freeboard Region above a Bubbling Fluidized Bed. Ind. Eng. Chem. Res., submitted.
14. Kaštánek P., Kaštánek F., Hájek M.: Microwave-enhanced Thermal Adsorption of Polyhalogenated Biphenyls from Contaminated Soil. J. Hazard. Mater., submitted.
15. Kaštánek F., Kaštánek P., Maléterová Y.: Dechlorination of PCBs in Aqueous Mixtures with Zero-Valent Iron in Statu Nascendi. Influence of Microwaves on the Rate of Reaction. J. Hazard. Mater., submitted.
16. Kment Š., Klusoň P., Hubička Z., Krýsa J., Čada M., Gregora I., Deyneka A., Remes Z., Žabová H., Jastrabík L.: Double Hollow Cathode Plasma Jet -Low Temperature Method for the TiO_2-xN_x Photoresponding Films. Electrochim. Acta, in press.

17. Martinec J., Šen H., Svoboda K., Martincová J.V., Baxter D.: The Thermal Protection of a Specific Experimental Instrument for Monitoring of Combustion Conditions on the Grate of Municipal Solid Waste Incinerators. Appl. Therm. Eng., submitted.
18. Pohořelý M., Jeremiáš M., Skoblia S., Vosecký M., Kameníková P., Šyc M., Tošnarová M., Punčochář M., Svoboda K.: Alotermní fluidní zplyňování biomasy. (Czech) Allothermal Fluidized Bed Biomass Gasification. Paliva 1, 23-30 (2010).
19. Šyc M., Pohořelý M., Kameníková P., Habart J., Punčochář M.: Willow Trees from Heavy Metals Phytoextraction as Energy Crops. Biomass and Bioenergy, submitted.

Review papers

20. Svoboda K., Martinec J., Pohořelý M., Baxter D.: Integration of Biomass Drying with Combustion/Gasification Technologies and Minimization of Emissions of Organic Compounds. Chem. Pap. 63(1), 15-25 (2009).
21. Svoboda K., Pohořelý M., Hartman M., Martinec J.: Pretreatment and Feeding of Biomass for Pressurized Entrained Flow Gasification. Fuel Process. Technol. 90(5), 629-635 (2009).

Chapters in books

22. Církva V., Žabová H.: Thin Nanoporous Titania Films on the Electrodeless Discharge Lamps for Photocatalysis. In: Handbook of Photocatalysts: Preparation, Structure and Applications. (Castello, G.K., Ed.), Nova Science Publishers, New York, in press.
23. Šyc M., Pekárek V., Novák P., Šolcová O., Pohořelý M., Punčochář M., Ocelka T.: Fly Ash Properties, Disposal, and Treatment in Modernized Waste Incineration Plant with Catalytic Filter. In: Fly Ash: Reuse, Environmental Problems and Related Issues. (Telone, P.H., Ed.), Nova Science Publishers, New York, in press.

Patents

24. Gruber V.: Method of Extraction of Europium(III) and/or Yttrium(III) Ions from Concentrate of Luminophore Dust or Sludge. Pat. No. EP 1817437/PCT/CZ2005/000088. Applied: 05.11.24, Patented: 09.03.25.
25. Novák L., Černín A., Hanika J., Veselý V.: Způsob a zařízení pro izolaci kyseliny tereftalové. (Czech) Princip and Device for Terephthalic Acid Isolation. Pat. No. PV 2008-602/CZ 301168. Applied: 08.10.09, Patented: 09.10.15.
26. Veselý V., Drahoš J., Šírek M.: Způsob chemické recyklace odpadního polyethylentereftelátu. (Czech) Waste PET Chemical Recycling. Pat. No. PV 2006-550/CZ 301118. Applied: 06.09.08, Patented: 09.10.02.
27. Hájek M., Sobek J., Brustman J.: Method for the Chemical Depolymerization of Waste Polyethylene Terephthalate. Pat. No. PCT/EP/2008/058917. Applied: 08.07.09.
28. Punčochář M., Skoblia S., Kameníková P.: Způsob stanovení celkového obsahu dehtu v plynu produkovaném zplyňováním paliva. (Czech) Method of Total Tar Content Determination in Gasifier Gas. Pat. No. PV 2008-780. Applied: 08.12.08.

International conferences

29. Bradová M., Hanika J., Veselý V.: Čištění tereftalátu membránovou technologií. (Czech) Terephthalate Purification by Membrane Technology. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 104, Srní, Šumava, Czech Republic, 19-22 October 2009.
30. Hájek M., Durovič M., Paulusová H., Weberová L.: Microwave Drying and Disinfection of Paper Documents. Water Impact on Library, Archival and Museum Materials, pp. 1-6, Praha, Czech Republic, 29-31 October 2009.
31. Hájek M., Sobek J.: Low Energy Depolymerization of Waste Polyethylene Terephthalate (PET). 2nd International Congress on Green Process Engineering, Proceedings, Venice, Italy, 14-17 June 2009.
32. Hanika J., Lederer J., Nečesaný F., Tukač V., Veselý V.: Možnosti produkce vodíku parciální oxidací odpadní biomasy. (Czech) Possibility of Hydrogen Production by Partial Oxidation of Waste Biomass. Seminář Biopaliva v dopravě, Book of Abstracts, 8 pp. full text on CD-ROM, Bratislava, Slovakia, 21-22 September 2009.

33. Hanika J., Lederer J., Nečesaný F., Tukač V., Veselý V.: Produkce vodíku současnou parciální oxidací odpadní biomasy a ropných zbytků. (Czech) Hydrogen Production by Partial Oxidation of Biomass and Crude Oil Wastes. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 48 (10 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
34. Hartman M., Trnka O., Svoboda K., Pohořelý M.: Evaluation of Fluidization Quality by Time-Series of Pressure Fluctuations. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 271 (17 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
35. Hopan F., Horák J., Dej M., Krpec K., Šyc M., Ocelka T., Tomšej T., Pekárek V.: Emission Factors of Pollutants from the Combustion of Brown Coal in Domestic Appliances. 29th International Symposium on Halogenated Persistent Organic Pollutants (Dioxin 2009), Organohalogen Compounds, Vol. 71, pp. 000715-718, Beijing, China, 23-28 August 2009.
36. Hopan F., Horák J., Šyc M., Krpec K., Dej M., Tomšej T., Ocelka T.: Srovnání produkce dioxinů a furanů pro různá paliva spalovaná v 25 kW automatickém kotli. (Czech) Comparison of PCDD/F Formation for Different Fuels Combusted in Automatic Boiler. Ochrana Ovzdušia 2009, Zborník , pp. 118-121, Štrbské Pleso, Slovakia, 25-27 November 2009.
37. Jeremiáš M., Pohořelý M., Vosecký M., Skoblia S., Kameníková P., Svoboda K., Punčochář M.: Experimental Study of Fluidized-Bed Biomass Gasification with CO_2+H_2O Mixtures on Limestone and Silica Sand. Clean Coal Technologies 2009, Proceedings, 12 pp. full text on CD-ROM, Dresden, Germany, 18-21 May 2009.
38. Jeremiáš M., Pohořelý M., Vosecký M., Skoblia S., Kameníková P., Svoboda K., Punčochář M.: The Influence of Addition of Carbon Dioxide to the Gasification Medium during the Atmospheric Steam Fluidized Bed Gasification on Sand and Limestone. Energetika a biomasa 2009, Sborník přednášek, pp. 80-93, Praha, Czech Republic, 18-19 February 2009.
39. Kaštánek P., Kaštánek F., Hájek M., Sobek J., Šolcová O.: Dechlorination of Polychlorinated Biphenyl (PCB) in Contaminated Soils and Oils. 11th International Conference on Environmental Science and Technology - CEST 2009, Volume of Abstracts, p. 76, Chania, Kréta, Greece, 03-05 September 2009.
40. Pohořelý M., Šyc M., Jeremiáš M., Vosecký M., Kameníková P., Skoblia S., Svoboda K., Punčochář M.: Fluidní zplyňování lnu z fytoextrakce těžkých kovů. (Czech) Fluidized Bed Gasification of Flax used for Phytoextraction of Heavy Metals. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 49 (10 pp. full text on CD-ROM), Srní, Šumava, Czech Republic, 19-22 October 2009.
41. Sobek J., Hájek M.: Alkylation of Aromatics by Alkenes in the Microwave Field. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 118, Tatranské Matliare, Slovakia, 25-29 May 2009.
42. Svoboda K., Pohořelý M., Hartman M., Punčochář M.: Possibilities of Carbon Dioxide Capture by Using Dry Soda Based Regenerable Sorbents. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 157 (9 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
43. Svoboda K., Punčochář M.: Czech Approach to Clean Power Generation, Reduction of CO_2 Emissions, and Exploitation of Renewable Sources of Energy. International Workshop Co-Gasification of Coal, Biomass and Waste, Workshop Abstracts, p. 16, Madrid, Spain, 12-13 November 2009.
44. Svoboda K., Šolcová O., Pohořelý M., Hartman M.: Enhanced Coalbed Methane Recovery by Means of Carbon Dioxide. 36th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 261 (15 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 25-29 May 2009.
45. Šyc M., Horák J., Hopan F., Dej M., Krpec K., Ocelka T., Tomšej T., Pekárek V.: Emission Factors of Selected Organic Compounds from Domestic Hardwood Combustion. 29th International Symposium on Halogenated Persistent Organic Pollutants (Dioxin 2009), Organohalogen Compounds, Vol. 71, pp. 000154-157, Beijing, China, 23-28 August 2009.
46. Šyc M., Pohořelý M., Kameníková P., Vosecký M., Punčochář M.: Possibilities of Contaminated Flax Utilization for Energetic Purposes. 10th International Conference on the Biochemistry of Trace Elements, Chihuahua, Mexico, 13-18 July 2009.
47. Taubner T., Sobek J., Havelka P., Kvasnička F., Synytsya A., Čopíková J.: Derivatives of Oxidized Cellulose. 5th International Conference on Polysaccharides-Glycoscience 2009, Chemické Listy 103(9), 777 p., 2009, Praha, Czech Republic, 11-13 November 2009.
48. Tlustoš P., Száková J., Balík J., Habart J., Pavlíková D., Punčochář M., Najmanová J.: Remediation Ability of Trees and Hyperaccumulators for Heavy Metals in Pot and Field Growing Conditions. 10th International Conference on the Biochemistry of Trace Elements, Chihuahua, Mexico, 13-18 July 2009.
49. Tukač V., Tomešová Z., Hanika J., Veselý V., Lederer J., Nečesaný F.: Možnosti produkce vodíku parciální oxidací odpadní biomasy. (Czech) Potential Hydrogen Production by Partial Oxidation of Waste Biomass. 18. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa .

Prostředí . Bezpečnost . APROCHEM 2008, Sborník přednášek, pp. 1140-1147, Milovy, Czech Republic, 20-22 April 2009.

50. Veselý V., Hanika J.: Ekonomika chemické recyklace PET lahví. (Czech) Economics of PET Bottles Chemical Recycling. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 51, Srní, Šumava, Czech Republic, 19-22 October 2009.
51. Vosecký M., Kameníková P., Pohořelý M., Skoblia S., Punčochář M.: Novel Approach to Tar Removal from Biomass Producer Gas by Means of a Nickel-based Catalyst. 20th International Conference on Fluidized Bed Combustion, Proceedings , pp. 740-746, Xi'an, China, 18-21 May 2009.
52. Vosecký M., Kameníková P., Pohořelý M., Skoblia S., Punčochář M.: Efficient Tar Removal from Biomass Producer Gas at Moderate Temperatures via Steam Reforming on Nickel-based Catalyst. 17th European Biomass Conference and Exhibition, Proceedings, pp. 862-866, Hamburg, Germany, 29 June - 03 July 2009.
53. Vosecký M., Skoblia S., Jirátová K., Kameníková P., Pohořelý M., Punčochář M.: Identification of Carbon Deposits on the Nickel-Based Catalyst used for the Steam Reforming of Biomass Tar at 500 °C. EuropaCatIX: "Catalysis for a Sustainable World", Abstracts p. 419 (2 pp. full text on CD-ROM), Salamanca, Spain, 30 August - 04 September 2009.
54. Žabová H., Církva V.: Preparation and Characterization of TiO_2 and Mn^{+}/TiO_2 and Their Utilization in Microwave Assisted Photocatalytic Reactions. 2nd China-Japan Symposium on Advanced Photocatalytic Materials (CJSAPM 2009), Program and Abstracts, pp. 54-55 (O-17), Nanjing, China, 05-07 March 2009.

Laboratory of Aerosol Chemistry and Physics

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Fields of research

- Composition, size and hygroscopicity of atmospheric aerosols
- Indoor/outdoor aerosols
- Nucleation phenomena
- Synthesis of nanoparticles *via* aerosol processes
- Heat and mass transfer in aerosol systems
- Interaction of aerosols with electromagnetic radiation
- Combustion aerosols
- Emissions sampling

Research projects

European supersites for atmospheric aerosol research
(J. Smolík, 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.

European integrated project on aerosol cloud climate and air quality interactions
(J. Smolík, supported by EC, project No. FP6-036833-2-EUCAARI)

European infrastructure project EUCAARI is designed as a research chain that aims to advance our understanding of climate and air quality through a series of connected activities beginning at the molecular scale and finishing at the regional and global scale. EUCAARI will build upon the pool of available data from previous field campaigns and long-term measurements in order to establish globally consistent data sets. A hierarchy of complementary models, at the molecular, process, meso-, regional and the global scale will be applied in a coordinated way in EUCAARI. [Ref. 23]

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

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

The aim of the project is to improve the characterization of PM10 suspended particles with the focus on secondary particle contribution, proposal of chemical model of secondary particles formation, identification of sources, and application and verification of dispersion models. The project provides direct support to the improvement of ambient air quality in the Czech Republic, respects the principle of air pollution prevention and meets the conception of sustainable development. [Refs. 43-45, 48, 54]

Evaluation of dynamics of aerosol particles in indoor environment

(J. Smolík, joint project with CTU, supported by GACR, grant No. GA101/07/1361)

The aim of the proposed project is to study experimentally the behaviour of aerosol particles in three different indoor environments: a full-scale laboratory room, unfurnished room in an apartment, and whole furnished apartment and to compare experimental results with theoretical predictions according to zonal mass-balance (MC-SIAM) and CFD (Fluent/FPM) modelling. The measurements will be done both under well-defined laboratory conditions (simple geometry, defined indoor boundary conditions, laboratory generated aerosol with narrow size distribution) and "real" conditions (furnished and/or unfurnished rooms, aerosol from different typical activities indoors, air exchange between indoor and outdoor environment and between compartments indoors). The purpose of the study is to test applicability of zonal mass-balance and CFD modelling and simulation for the prediction of indoor aerosol dynamics. [Refs. 3, 4, 14, 40]

Similarities and differences of ultrafine urban aerosol in Budapest and Prague

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

The main objectives of the project are to determine the concentrations, size distributions and other relevant properties of the ultrafine aerosol particles in Budapest and Prague, to intercompare the measuring results and conclusions for both capitals in order to identify general properties and specialities, to assess the relationships between the size distribution and deposition in the human respiratory system for the ultrafine aerosol, and to study the dynamics of the new aerosol particle formation and growth including specialities in Budapest and Prague. [Ref. 45]

Composite nanoparticle synthesis by an aerosol process

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

Project involves an experimental study of nanoparticle synthesis by chemical vapour condensation method in an externally heated tube flow reactor. In the first part of the project: (i) single component metal and ceramic particles (Co, Ni, Pd, MnO) with great potential of applications will be prepared by thermal decomposition of corresponding metal-organic compounds. In the next step: (ii) binary mixed or coated metal-ceramic particles (TiO_2-Co, Al_2O_3-Ni, Al_2O_3-Pd) with potential use as catalyst and binary metal-ceramic (Co-SiO_2) and ceramic-ceramic (MnO-SiO_2) particles with potential applications as gas sensors or in electronics will be prepared by simultaneous decomposition of two precursors. Particle morphology, crystallinity, and chemical composition will be examined by SEM, TEM, SAED, XRD, EDS, etc. Results obtained in a hot wall reactor will be compared with those

from experiments with liquid flame spray reactor at Tampere University of Technology. [Refs. 8, 16, 26-33, 37]

Friction materials based on polymer matrix containing metals and their impact on environment

(P. Moravec, joint project with TU Ostrava, and Southern Illinois University, US, supported by GACR, grant No. GA106/07/1436)

The project focuses on study of friction processes of laboratory prepared friction materials and original brake samples; further on structure identification of micro- and nanoscale wear particles with a view to reduce adverse anthropogenic impacts related to wear debris generation and deposition on the environment. An interdisciplinary and international CZE-US team consisting of researchers in the areas of materials science, chemistry, toxicology, medicine, and aerosol science will address the fundamental understanding of comprehensive material flow related to braking operations. The proposed research based on interconnection of material analyses and toxicological assessment (ecotoxicity, genotoxicity, and pulmonary toxicity) will allow identification of undesirable components in automotive friction materials and prediction of the environmental impact of wear particles release from brakes. [Ref. 38]

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

(V.V. Levdanski, supported by AS CR, 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. 5-8, 16, 25-34]

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

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

The aim of the proposed project is to suggest possible legal measures to decrease level of atmospheric aerosol burden in the Czech Republic. The sampling and chemical analysis of both particulate emissions and immissions at several types of sources and places in the Czech Republic, statistical analysis of the results and toxicological characterization of particles will be used to fulfill the aim of the project. [Refs. 47, 49]

Chemical interactions between cultural artefacts and indoor environment (EnviArt)

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

The aim of EnviArt is to explore chemical interactions between cultural artefacts and typical indoor environmental conditions through field studies and laboratory experiments and transfer the results into preventive conservation practice. The Action focuses on the chemical

impact of pollutants on materials, thus also considering physical and environmental aspects, materials technology, chemical analytics, emission and standardization.

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

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

The main goal of the project is detailed characterization of indoor air pollution in the Baroque Library Hall of the National Library Hall in Prague. The research is focused both on gaseous pollutants and particulate matter (PM), including the estimation of outdoor and indoor sources contribution. [Refs. 41, 42]

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

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

The aim of the project is detailed characterization of size-resolved PM in the indoor environment of the National Library in Prague, with possible effects on deposited books and manuscripts and estimation of contribution of typical activities indoors [Refs. 41, 42].

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

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

The objectives of project can be summarized as follows: Atmospheric aerosol elemental composition on daily based samples 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. [Ref. 53]

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

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

The aim of the project is to determine some properties of heterogeneous nuclei present in the superheated steam of steam turbines. In this project, the sampling device, coupled to advanced aerosol instrumentation (condensation particle counter, scanning mobility particle sizer), 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. 6, 24-30, 33, 34]

Thermophysical properties of water in unexplored, technologically significant regions
(V. Ždímal, joint project with Institute of Thermomechanics of the ASCR, v. v. i., CTU, and University of West Bohemia, Plzeň, supported by ASCR, grant No. IAA4200760905)

This project 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. 1, 5, 6, 19, 25, 31, 34, 52, 57]

New ways to synthesize nanoparticles of various oxides
(V. Ždímal, joint project with the ICT and Spolchemie, supported by the MIT-FR, grant No. FR-TI1/548, 2009-2012)

The aim of the project is to seek new ways how to synthesize nanoparticles of various oxides, characterize produced particles and perform a process scale–up.

International co-operations

Philipps-University Marburg, Marburg, Germany: Experimental study of homogeneous nucleation in supersaturated vapours
Finnish Meteorological Institute, Helsinki, Finland: Studies on homogeneous nucleation using diffusion chambers
Norwegian Institute for Air Research, Kjeller, Norway: Indoor aerosol behaviour
Technical University of Crete, Chania, Greece: Aerosols in the environment
Tampere University of Technology, Tampere, Finland: Synthesis and characterization of nanosized metal/ceramic particles
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
Southern Illinois University, Carbondale, USA: Friction materials based on polymer matrix containing metals and their impact on environment
Division of Nuclear Physics, Department of Physics, Lund University, Lund, Sweden
Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, Switzerland
Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan
University of Helsinki, Division of Atmospheric Sciences, Helsinki, Finland

Visits abroad

J. Ondráček: Institute of Environmental Engineering, National Chiao Tung University, Hsinchu, Taiwan (1 month)

Visitors

T. Hussein, University of Helsinki, Helsinki, Finland
V. Nororos, University of Helsinki, Helsinki, Finland

Teaching

V. Ždímal: Faculty of Mathematics and Physics, CU, postgraduate course: "Aerosol Engineering"

Publications

Original papers

1. Brus D., Ždímal V., Uchtmann H.: Homogeneous Nucleation Rate Measurements in Supersaturated Water Vapor II. J. Chem. Phys. 131(7), 074507: 1-9 (2009).
2. Herrmann E., Hyvärinen A.-P., Brus D., Lihavainen H., Kulmala M.: Re-evaluation of the Pressure Effect for Nucleation in Laminar Flow Diffusion Chamber Experiments with Fluent and the Fine Particle Model. J. Phys. Chem. A 113(8), 1434-1439 (2009).
3. Hussein T., Hruška A., Dohányosová P., Džumbová L., Hemerka J., Kulmala M., Smolík J.: Deposition Rates on Smooth Surfaces and Coagulation of Aerosol Particles Inside a Test Chamber. Atmos. Environ. 43(4), 905-914 (2009).
4. Hussein T., Kubincová L., Džumbová L., Hruška A., Dohányosová P., Hemerka J., Smolík J.: Deposition of Aerosol Particles on Rough Surfaces Inside a Test Chamber. Build. Environ. 44(10), 2056-2063 (2009).
5. Levdansky V.V., Dragun V.L., Smolík J., Moravec P.: Vliyanie poverkhnostnykh protsessov na techenie gazov v nanorazmernykh kapillyarakh. (Russ). Vestsi Nat. Ak. Nauk Belarusi, Ser. Fyz.-Tekh. Navuk 2, 69-73 (2009).
6. Levdansky V.V., Smolík J., Moravec P.: Kriticheskii razmer aerozoľnykh chastits pri fizicheskom a khimicheskom osazhdenii. (Russ). Inzh. - Fiz. Zh. [J. Eng. Phys. Thermophys. 82(4), 649-656, 2009] 82(4), 656-662 (2009).
7. Levdansky V.V., Smolík J., Moravec P.: Radiation-induced Mass Transfer through Membranes. Int. Commun. Heat Mass Transfer 36(2), 125-128 (2009).
8. Levdansky V.V., Smolík J., Moravec P.: Impurity Trapping by Aerosol Particles. Aerosol Air Quality Res. 9(2), 257-265 (2009).
9. Ondráček J., Ždímal V., Smolík J., Lazaridis M.: A Merging Algorithm for Aerosol Size Distribution from Multiple Instruments. Water Air Soil Pollut. 199(1-4), 219-233 (2009).
10. Smolík J., Bízek V., Schwarz J., Ždímal V., Ondráček J., Ondráčková L., Andělová L.: Příspěvek automobilové dopravy k místnímu znečištění ovzduší. (Czech) Contribution of Vehicle Traffic to Local Air Pollution. Ochrana ovzduší 21(41)(3), 21-26 (2009).
11. Chen S.-Ch., Tsai Ch.-J., Huang Ch.-Yu, Chen H.-D., Chen S.-J., Lin Ch.-Ch., Tsai J.-H., Chou Ch.C.K., Lung S.-Ch., Huang W.-Ru, Smolík J., Džumbová L.: Chemical Mass Closure and Chemical Characteristics of Ambient PM0.1, PM2.5 and PM10 in a Highway Tunnel and at a Roadside. Aerosol Sci. Technol., in press.
12. Moravec P., Smolík J., Keskinen H., Mäkelä J.M., Bakardjieva S., Levdansky V.V.: NiOx Nanoparticle Synthesis by Chemical Vapor Deposition from Nickel Acetylacetonate. Aerosol Air Qual. Res., submitted.
13. Putaud J-P., Van Dingenen R., Alastuey A., Bauer H., Birmili W., Cyrys J., Flentje H., Fuzzi S., Gehrig R., Harrison R.M., Schwarz J., Smolík J.: A European Aerosol Phenomenology - 3: Physical and Chemical 2 Characteristics of Particulate Matter from 60 Rural, Urban, and Kerbside Sites Across Europe. Atmos. Environ., in press.
14. Smolík J., Ondráčková L., Maršíková J.: Koncentrace aerosolových částic v zubní ordinaci. (Czech) Aerosol Particle Concentration in a Dental Office. Chem. Listy, submitted.
15. Štefancová L., Schwarz J., Maenhaut W., Chi X.: Hygroscopic Growth of Atmospheric Aerosol Sampled in Prague 2008 Using Humidity Controlled Inlets. Atmospheric Research, submitted.

Chapters in books

16. Levdansky V.V., Dragun V.L., Smolík J., Moravec P.: Upravlenie geterogennymi protsessami v tonkikh kanalakh (kapillyarakh) i poristykh telakh. (Russ). In: Teplo- i Massoperenos - 2008. (Dragun, V.L., Ed.), pp. 163-167, Institut teplo- i massoobmena A.V. Lykova, Minsk 2009.

International conferences

17. Biskos J.G., Vratolis S., Ondráček J., Karanasiou A.A., Eleftheriadis K.: Volatility of Nuclei Mode Arctic Aerosol Particles during Summer. European Aerosol Conference 2009, Program and Abstracts, T160A13, Karlsruhe, Germany, 06-11 September 2009.
18. Brus D., Hyvärinen A., Lihavainen H., Kulmala M.: Binary Homogeneous Nucleation of H_2SO_4-H_2O. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 659-662, Prague, Czech Republic, 10-14 August 2009.
19. Brus D., Ždímal V., Uchtmann H.: Nucleation Behavior of Sulfur Vapor Reinvestigated by an Improved Experimental Technique. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 484-487, Prague, Czech Republic, 10-14 August 2009.
20. Eleftheriadis K., Vratolis S., Karanasioy A.A., Biskos J.G., Ondráček J.: Volatility of Nuclei Mode Arctic Aerosol. 19th Annual VM Goldschmidt Conference, Geochimica at Cosmochimica Acta 73(13), A324, 2009, Davos, Switzerland, 21-26 June 2009.
21. Hyvärinen A.-P., Wedekind J., Brus D., Lihavainen H.: Carrier Gas Pressure Effect in Homogeneous Nucleation of n-Alcohols. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 642-645, Prague, Czech Republic, 10-14 August 2009.
22. Chen S.C., Tsai C.J., Chen S.J., Lin C.C., Chou Ch.C.K., Lung S.C., Roam G.D., Wu W.Y., Smolík J., Džumbová L.: Environmental Ultrafine, Fine and Coarse Particles in a Highway Tunnel and at a Roadside. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 200-203, Prague, Czech Republic, 10-14 August 2009.
23. Kerminen V.-M., Lihavainen H., Brus D., Asmil E., Sipilä M., Manninen H.E., Kurten T., Vehkamäki H., Ortega I.K., Mirme A., Mirme S., Uin J.: Nucleation Studies within the EUCAARI Project. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 322-325, Prague, Czech Republic, 10-14 August 2009.
24. Kovářová E., Ždímal V.: Depozice inhalantů v dýchacím ústrojí člověka. (Czech) Deposition of Inhalants in the Human Respiratory Tract. X. konference České aerosolové společnosti, Sborník konference, pp. 59-60, Čejkovice, Czech Republic, 12-13 November 2009.
25. Levdansky V.V., Smolík J., Moravec P.: Size Effect in Phase Transitions in Aerosol Systems with Nanoscale Particles (Clusters). X. konference České aerosolové společnosti, Sborník konference, pp. 73-74, Čejkovice, Czech Republic, 12-13 November 2009.
26. Levdansky V.V., Smolík J., Moravec P.: Size Effects in Coalescence of Nanoscale Aerosol Particles. X. konference České aerosolové společnosti, Sborník konference, pp. 75-76, Čejkovice, Czech Republic, 12-13 November 2009.
27. Levdansky V.V., Smolík J., Moravec P.: Diffusion of Gases in Porous Membranes in Field of Resonance Radiation. DSL 2009, Abstracts Book, p. 202, Rome, Italy, 24-26 June 2009.
28. Levdansky V.V., Smolík J., Moravec P.: Gas Pumping Through Membranes by Resonance Radiation. 17th International Conference on Advanced Laser Technologies, Book of Abstracts, p. 228, Antalya, Turkey, 26 September - 01 October 2009.
29. Levdansky V.V., Smolík J., Moravec P.: Critical Size of Charged Aerosol Particles in the Presence of Adsorbable Foreign Gas. European Aerosol Conference 2009, Program and Abstracts, T071A02, Karlsruhe, Germany, 06-11 September 2009.
30. Levdansky V.V., Smolík J., Moravec P.: Gas Flow in Nanoporous Membranes. 3rd International Symposium Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 137, Albena, Bulgaria, 06-09 September 2009.
31. Levdansky V.V., Smolík J., Moravec P.: Influence of Size Effect, Resonance Radiation and Surface Processes on Critical Diameter of Aerosol Particles. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 630-633, Prague, Czech Republic, 10-14 August 2009.
32. Levdansky V.V., Smolík J., Moravec P.: Size Effect in Chemical Reactions in Nanoparticles. International Conference Nanomeeting 2009, Proceedings, pp. 442-445, Minsk, Belarus, 26-29 May 2009.
33. Levdansky V.V., Smolík J., Moravec P.: Thin Film Deposition on Inner Surface of Porous Body. E-MRS 2009 Spring Meeting, Book of Abstracts, p. PP9 3, Strasbourg, France, 08-12 June 2009.

34. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Effect of Surface Phenomena in Condensation of Molecules on Small Charged Aerosol Particles. XIIIth Research Workshop Nucleation Theory and Applications, Invited lecture, Dubna, Russia, 01 April 2009 - 30 April 2008.
35. Manka A., Brus D., Hyvärinen A.-P., Lihavainen H., Wölk J., Strey R.: Homogeneous Water Nucleation in a Laminar Flow Diffusion Chamber. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 480-483, Prague, Czech Republic, 10-14 August 2009.
36. Manka A., Brus D., Hyvärinen A.-P., Lihavainen H., Wölk J., Strey R.: Homogeneous Water Nucleation in a Laminar Flow Diffusion Chamber. European Aerosol Conference 2009, Program and Abstracts, T032A02, Karlsruhe, Germany, 06-11 September 2009.
37. Moravec P., Smolík J., Levdansky V.V., Klementová M.: Composite CuO_x-SiO_2 Nanoparticle Synthesis by MOCVD. European Aerosol Conference 2009, Program and Abstracts, T015A29, Karlsruhe, Germany, 06-11 September 2009.
38. Moravec P., Smolík J., Schwarz J., Ševčíková I., Kukutschová J., Tomášek V.: Sampling and Characterization of Airborne Particle from Car Brakes Testing. X. konference České aerosolové společnosti, Sborník konference, pp. 25-30, Čejkovice, Czech Republic, 12-13 November 2009.
39. Neitola K., Brus D., Sipilä M., Kulmala M.: Particle Size Dependence on Sulphuric Acid Concentration in Binary Homogeneous Nucleation of H_2SO_4-H_2O System. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 655-658, Prague, Czech Republic, 10-14 August 2009.
40. Ondráček J., Brand M., Barták M., Džumbová L., Smolík J.: Behaviour of Well Defined Aerosol Particles in a Test Chamber. European Aerosol Conference 2009, Program and Abstracts, T108A13, Karlsruhe, Germany, 06-11 September 2009.
41. Ondráčková L., Ondráček J., Andělová L., Smolík J.: Koncentrace aerosolu v barokním knihovním sále Národní knihovny. (Czech) Measurement of Aerosol Particles Concentration in Baroque Library Hall of National Library. X. konference České aerosolové společnosti, Sborník konference, pp. 9-10, Čejkovice, Czech Republic, 12-13 November 2009.
42. Ondráčková L., Smolík J.: Aerosol Particles in the Baroque Library Hall of the National Library in Prague. European Aerosol Conference 2009, Program and Abstracts, T108A10, Karlsruhe, Germany, 06-11 September 2009.
43. Řimnáčová D., Borsós T., Ždímal V., Salma I., Schwarz J., Smolík J.: Comparison of Ultrafine Atmospheric Aerosols in Prague and Budapest. X. konference České aerosolové společnosti, Sborník konference, pp. 11-14, Čejkovice, Czech Republic, 12-13 November 2009.
44. Řimnáčová D., Ždímal V., Schwarz J., Smolík J.: Dynamics of Atmospheric Aerosol Particle Size Distributions at Prague Suburbs. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 845-848, Prague, Czech Republic, 10-14 August 2009.
45. Řimnáčová D., Ždímal V., Schwarz J., Smolík J.: Atmospheric Aerosols in the Suburb of Prague. European Aerosol Conference 2009, Program and Abstracts, T051A30, Karlsruhe, Germany, 06-11 September 2009.
46. Schwarz J., Havránek V., Maenhaut W., Chi X., Ždímal V., Hovorka J., Smolík J.: Properties and Sources of Suburban Background Atmospheric Aerosol in Prague. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 188-191, Prague, Czech Republic, 10-14 August 2009.
47. Schwarz J., Vodička P.: Tuning of Sunset EC/OC Field Instruments to Obtain More than Comparable Data. European Aerosol Conference 2009, Program and Abstracts, T150A29, Karlsruhe, Germany, 06-11 September 2009.
48. Schwarz J., Vodička P., Smolík J.: Organic and Elemental Carbon with a Higher Time Resolution in the PM2.5 Fraction in Prague Suchdol. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 866-869, Prague, Czech Republic, 10-14 August 2009.
49. Schwarz J., Vodička P., Smolík J.: Organický a elementární uhlík s vyšším časovým rozlišením ve frakci PM2,5 v Praze Suchdole: první výsledky ze zimní kampaně. (Czech) Organic and Elemental Carbon with a Higher Time Resolution in the PM2.5 Fraction in Prague Suchdol. Ovzduší 2009, Program a sborník konference, pp. 245-248, Brno, Czech Republic, 26-29 April 2009.
50. Smolík J., Bízek V., Schwarz J., Ždímal V., Ondráček J., Ondráčková L., Andělová L.: Příspěvek dopravy k místnímu znečištění ovzduší. (Czech) Traffic Contribution to the Local Air Pollution. Ozduší 2009, Program a sborník konference, pp 62-66, Brno, Czech Republic, 26-29 April 2009.
51. Štefancová L., Schwarz J., Maenhaut W., Chi X., Smolík J.: Chemical Size Distribution of Suburban Aerosol Sampled in Prague 2008 Using Humidity Controlled Inlets. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 155-158, Prague, Czech Republic, 10-14 August 2009.

52. Uchtmann H., Brus D., Ždímal V.: A Comparative Study of Homogeneous Nucleation Rate Measurements in Thermal Diffusion Cloud Chambers. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 476-479, Prague, Czech Republic, 10-14 August 2009.
53. Vodička P., Schwarz J., Smolík J.: Analýza elementárního a organického uhlíku v aerosolech: křižovatka vs. zástavba. (Czech) Analysis of Elemental and Organic Carbon Aerosols: Crossroad vs. Suburban Area. X. konference České aerosolové společnosti, Sborník konference, pp. 19-22, Čejkovice, Czech Republic, 12-13 November 2009.
54. Wagner Z., Schwarz J., Ždímal V., Eleftheriadis K., Lazaridis M., Smolík J.: Analysis of Time Evolution of Particle Size Distribution. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 116-119, Prague, Czech Republic, 10-14 August 2009.
55. Wedekind J., Hyvärinen A.-P., Brus D., Reguera D.: The Pressure-Effect in Unary Condensation. 18th International Conference Nucleation and Atmospheric Aerosols, Book of Abstracts, pp. 607-610, Prague, Czech Republic, 10-14 August 2009.
56. Wedekind J., Hyvärinen A.-P., Brus D., Reguera D.: Unrevealing the "Pressure-Effect" in Unary Condensation. European Aerosol Conference 2009, Program and Abstracts, T032A01, Karlsruhe, Germany, 06-11 September 2009.
57. Ždímal V., Uchtmann H., Brus D.: Srovnávací studie měření homogenní nukleace vody ve statických difúzních komorách. (Czech) A Comparison Study on Measurements of Homogeneous Nucleation Rate of Water in Static Diffusion Chambers. X. konference České aerosolové společnosti, Sborník konference, pp. 69-72, Čejkovice, Czech Republic, 12-13 November 2009.

Laboratory of Laser Chemistry

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Fields of research

- IR and UV laser induced chemistry
- Chemical vapour deposition of novel Si- , Ge- and C-based nanostructured materials
- IR laser-induced carbothermal reduction of oxides
- IR and UV laser photopolymerization in the gas phase
- UV laser chemical liquid deposition of metal nanosols and nanocomposites
- IR and UV laser induced ablation of polymers
- IR and UV laser deposition of TiO_2-based photocatalysts

Research projects

New laser induced process for production of novel carbon-based nanomaterials and carbon-based nanomaterials with incorporated Si, N, and B heteroatoms
(J. Pola, supported by ASCR, grant No. IAA400720619)

MW and GW UV laser-induced photolysis of gaseous benzene, toluene, pyridine and acetylene has been demonstrated as a process leading to transient polyacetylenes and cumulenes and yielding nanostructured carbon soot whose properties depend on the precursor. Simultaneous back-side etching of silica adjacent to laser-induced plasma enables to enrich the soot with polyoxocarbosilane. The process was previously shown as capable of chemical vapour deposition of composites containing nanodomains of very rare chaoite in amorphous C/Si/O/N phase, conversion of silica into nanosized carbon-polyoxocarbosilane composites, or deposition of for the first time prepared nanosized silicon oxycarbide. Our studies have been continuing in 2009 by exploration of (i) chemical vapour deposition of Co-C films through concurrent IR laser-induced ablation of metals and adjacent dielectric breakdown in gaseous hydrocarbons and (ii) studies on chemical vapour deposition of ultrafine Cl-substituted carbonaceous powders by using intense UV laser photolysis of dichloroethenes. The former process affords deposition of Co, Co_2C and Co_3C nanograins embedded in a shell of hexagonal graphite and amorphous sp^3-hybridized carbonaceous matrix, and the latter process results in deposition of novel nanoscopic Cl-substituted hydrogenated carbon that has a potential for structural modification of carbon materials at the C-Cl bonds. [Refs. 14, 16]

Green chalcogenation of metals by laser-prepared poly(silachalcogenide)
(J. Pola, supported by GACR, grant No. GA203/09/0931

IR and UV laser co-photolysis of silane and thiirane has been studied to explore chemical vapor deposition and reactivity of poly(silathiane) towards selected metal surfaces. The poly(silathiane) formation in the gas phase and deposition on metal surfaces was found out as a feasible process, but sulfidation of metal surfaces by this inorganic polymer reagent appears to be restricted to thin polymer-metal interphase and Cu and Bi only. Raman spectral studies confirm this conclusion. The experimental study was preceded by literature search and compiling the data on laser deposition of nanostructured Se- and Te-based materials. [Ref. 7]

IR Laser gas-phase deposition of metastable binary alloys from volatile Si, Ge and Sn precursors
(J. Pola, supported by ICPF)

IR laser-induced co-decomposition of binary gaseous mixtures of MH_4 and $M(CH_3)_4$ (M = Si, Ge, Sn) has been recognized as a novel process for gas-phase deposition of M elements alloys. The process is initiated in dielectric breakdown or by infrared multiple photon absorption in IR radiation absorbing gas and it involves extrusion and coalescence of M elements and cooling of their nanosized metastable alloys in the gas phase within short laser pulses. This one-step process represents a simple approach for synthesis of nanosized metastable alloys. [Refs. 5, 6, 12, 13]

Preparation of nanostructured Si/Ge/C deposits
(V. Dřínek, supported by GACR, grant No. GA203/09/1088)

Thermal decomposition of hexamethyldigermane led to formation of bare germanium nanowires. Strong influence of selected metal substrates on nanowire growth was established. Thermal evaporation of Ge on Si and SiO_2 substrates prior thermal decomposition initiated nanowire growth as well. The nanowires were several microns long and approximately 10 nm in diameter. Nanoplates were formed on copper sheets using precursor mixture of ethylsilane and hexamethyldigermane. The areas of nanoplates are up to thousands square microns and thickness about 50 nm. EDX analysis revealed $SiGe_x$ composition. Along with nanoplates, $SiGe_x$ nanowires were formed. [Refs. 2, 3, 9]

Laser decomposition of cobalt and nickel carbonyls in the presence of acetylene for preparation of carbon encapsulated metal nanoparticles
(R. Fajgar, supported by GA CR, grant No. GA203/07/0546)

Mixture of iron pentacarbonyl, cobalt tricarbonyl nitrosyl and acetylene decomposes under UV laser irradiation to form Co/Fe alloy nanoparticles encapsulated in carbon. As-prepared equiatomic Co Fe nanoparticles with diameter 5 nm, encapsulated in the amorphous carbon crystallize above 600^{o}C and form ordered alloys. Iron-rich alloys were prepared and the as-prepared samples are amorphous with randomly distributed cobalt atoms in iron. Heating of the deposited material leads to separation of the metals. XRD and Moessbauer analysis revealed formation of new ordered phases Fe_7Co and $Fe_{15}Co$. Magnetic measurements revealed strong superparamagnetic behaviour of the Co/Fe nanoparticles at temperatures up to 140 K. Carbon has a turbostratic structure with BET surface up to 290 m^2/g. [Refs. 4, 11]

Preparation of Ti/O/Si based photocatalysts by laser induced CVD and sol-gel technique
(R. Fajgar, supported by GACR, grant No. GA203/09/1117)

UV laser-induced deposition of chromium doped TiO_2/SiO_2 films from $TiCl_4/SiCl_4/CrO_2Cl_2$ mixtures was studied. The films, deposited on glass substrates were

annealed up to 600°C. Photocatalytic activity and hydrophilicity were studied. The films annealed at 500°C possess good adhesion to the glass substrate and revealed excellent superhydrophilic properties. TiO_2/SiO_2 nanoparticles were prepared by laser-induced oxidation of tetrakis(trimethylsiloxy) titanium. The oxidation shows an explosive course and direct formation of TiO_2 nanoparticles encapsulated in SiO_2 was observed. The nanoparticles with diameter up to 50 nm were studied and characterized by means of spectroscopy, microscopy and diffraction techniques.

International co-operations

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

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

National Institute of Advanced Industrial Research and Technology, Tsukuba, Japan: Laser control of organic reactions

University of Crete, Heraklion, Greece: Laser induced chemical vapour deposition of 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

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

POLYMAT, Institute for Polymer Materials, San Sebastian, Spain

Visitors

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Duong Ngoc Hai, Vietnam Academy of Science and Technology, Hanoi, Vietnam
Ninh Khac Ban, Vietnam Academy of Science and Technology, Hanoi, Vietnam

Publications

Original papers

1. Blazevska-Gilev J., Bastl Z., Šubrt J., Stopka P., Pola J.: IR Laser Ablative Degradation of Poly(phenylene ether sulfone): Deposition of Films Containing Sulfone, Sulfoxide and Sulfide Groups. Polym. Degrad. Stabil. 94(2), 196-200 (2009).
2. Dřínek V., Klementová M., Šubrt J.: Deposition of Germanium Nanowires from Digermane Precursor: Influence of the Substrate Pretreatment. Electrochem. Soc. Trans. 25(8), 1015-1022 (2009).
3. Dřínek V., Šubrt J., Klementová M., Rieder M., Fajgar R.: From Shelled Ge Nanowires to SiC Nanotubes. Nanotechnology 20(3), 035606 (2009).

4. Fajgar R., Bastl Z., Šubrt J., Murafa N., Maryško M.: ArF Laser-induced Deposition of Carbon Encapsulated Co Fe Nanoparticles. Electrochem. Soc. Trans. 25(8), 1023-1030 (2009).
5. Křenek T., Bezdička P., Murafa N., Šubrt J., Pola J.: Laser CVD of Nanodisperse Ge-Sn Alloys Obtained by Dielectric Breakdown of SnH4/GeH4 Mixtures. Eur. J. Inorg. Chem. 2009(11), 1464-1467 (2009).
6. Křenek T., Bezdička P., Murafa N., Šubrt N., Duchek P., Pola J.: IR Laser-induced CVD of beta-Sn/SnSi-Nanodisperse Alloys from Stannane–silane Mixture. J. Anal. Appl. Pyrolysis 86(2), 381-385 (2009).
7. Pola J., Ouchi A.: Laser Photolysis and Thermolysis of Organic Selenides and Tellurides for Chemical Gas-phase Deposition of Nanostructured Materials. Molecules 14(3), 1111-1125 (2009).
8. Daniloska V., Blazevska-Gilev J., Dimova V., Fajgar R., Tomovska R.: UV Light Induced Surface Modification of HDPE Films with Bioactive Compounds. Appl. Surf. Sci. 256(7), 2276-2283 (2010).
9. Dřínek V., Fajgar R., Klementová M., Šubrt J.: Deposition of Germanium Nanowires from Digermane Precursor: Influence of the Substrate Pretreatment. J. Electrochem. Soc., submitted.
10. Dřínek V., Vacek K.: IR Evidence of Peroxy Radical SiOO(˙). Appl. Phys. A: Solids Surf., submitted.
11. Fajgar R., Bastl Z., Šubrt J., Murafa N., Maryško M.: ArF Laser-induced Deposition of Carbon Encapsulated Co Fe Nanoparticles. J. Electrochem. Soc., submitted.
12. Křenek T., Murafa N., Bezdička P., Šubrt J., Pola J.: Laser-induced Dielectric Breakdown in Tetramethylgermane / Tetramethyltin Mixtures: Deposition of Nanostructured Sn/Ge/C and Ge-Sn/C Films. Appl. Organometal. Chem., in press.
13. Křenek T., Murafa N., Bezdička P., Šubrt J., Pola J.: IR Laser CVD of Nanostructured Si/Ge Alloy from Silane-Germane Mixture. J. Anal. Appl. Pyrolysis, submitted.
14. Pola J., Urbanová M., Pokorná D., Šubrt J., Bakardjieva S., Bezdička P., Bastl Z.: IR Laser-induced Formation of Amorphous Co-C Films with Crystalline Co, Co_2C and Co_3C Nanograins in a Graphitic Shell. J. Photochem. Photobiol., A, in press.
15. Santos M., Díaz L., Camacho J.J., Poyato J.M., Pola J., Křenek T.: Laser Induced Breakdown Spectroscopy of Germane Plasma Induced by IR CO_2 Pulsed Laser. J. Phys. B, submitted.
16. Santos M., Díaz L., Camacho J., Urbanová M., Pokorná D., Šubrt J., Bakardjieva S., Bastl Z., Pola J.: IR Laser-induced Metal Ablation and Dielectric Breakdown in Benzene. Infrared Phys. Technol. 53(1), 23-28 (2010).
17. Vacík J., Lavrentiev V., Novotná K., Bačáková L., Lisá V., Vorlíček V., Fajgar R.: Fullerene (C60)-Transitional Metal (Ti) Composites: Structural and Biological Properties of the Thin Films. Diam. Relat. Mater. 19(2-3), 242–246 (2010).

International conferences

18. Dřínek V., Fajgar R., Šubrt J., Klementová M.: Deposition of Germanium Nanowires from Digermane Precursor: Influence of the Substrate Pretreatment. 216th ECS Meeting, Meeting Abstracts, Abs.2621, Vienna, Austria, 04-09 October 2009.
19. Duchek P., Šabata S., Křenek T.: The Influence of Organic Modifier In a Commercially Available Organoclay on the Intercalation Process. International Conference on Advanced Nanomaterials and Nanotechnology ICANN 2009, p. 344 (D-240), Guwahati, India, 09-11 December 2009.
20. Fajgar R., Bastl Z., Šubrt J., Murafa N., Maryško M.: ArF Laser-induced Deposition of Carbon Encapsulated Co Fe Nanoparticles. 216th ECS Meeting, Meeting Abstracts, Abs.2622, Vienna, Austria, 04-09 October 2009.

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Fields of research

- NMR spectroscopy

Applied research

- Development of new analytical methods
- Analytical services to the research departments of ICPF

Research projects

Reactivity of asymmetrically substituted epimino pyranoses
(J. Karban, joint project with CU, supported by ASCR, grant No. IAA400720703)

We have finished our work on aziridine-ring cleavage of 4-deoxy-2,3-epimino derivatives of 1,6-anhydro-β-D-hexopyranoses. The regioselectivity of the cleavage was found to be governed by interplay of S_N2 and S_N2-borderline mechanism depending on the type of the nucleophile (hard versus soft) and conditions (acidic versus basic). To further investigate the cleavage mechanism we have prepared the full series of all configurational isomers of 4-fluoro-2,3-epimino-1,6-anhydro-β-D-hexopyranoses. These fluoro compounds were prepared by reaction of suitable azido sulfonates containing a free 4-hydroxyl with diethylaminosulfur trifluoride and subsequent reductive cyclization. The study of their reactivity is now in progress. [Refs. 5, 14, 20]

Structure of silyl moieties through J(^{29}Si-^{13}C) couplings as determined by triple {^{1}H, ^{13}C}^{29}Si NMR experiment
(J. Schraml, supported by ASCR, grant No. IAA400720706)

New methods for measurement of spin-spin couplings between ^{29}Si and ^{13}C nuclei in solutions utilize instrumental possibilities of triple resonance of ^{1}H-^{13}C-^{29}Si nuclei which enhance the sensitivity to the extent that expensive isotopic enrichment, common for bio-NMR, is not needed. The developed methods were extended to ^{15}N couplings [Ref. 4]. Using these experiments model series of compounds are measured and calculated [Refs. 1, 2] to

produce the dependence of the vicinal ^{29}Si-^{13}C couplings on dihedral angles and, subsequently, also the dependence on the nature of substituents [Refs. 17, 18, 29].

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

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

Project objective is to evolve generally applicable NMR method for structural analysis of branched siloxanes based on Si-Si connectivity. Besides the well-known methods, new pulse sequences employing gradient and shaped pulses will be developed. The first experiments are conducted on commercially available model compounds; in later phase of project series of models will be synthesized. The research will advance from simple linear and branched oligosiloxanes towards to more complex macromolecules. Simultaneously, developed methods are adapting for HPLC analysis of organosilicon polymers and copolymers with ^{29}Si NMR detection in stop-flow mode. [Refs. 21, 22]

Dehydrocoupling reactions catalyzed by titanium complexes

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

The project deals with the reactivity of titanium catalytic systems toward hydrogen-main group element bond (H-E) mainly in silanes (primary, secondary). The catalytic reaction leads to formation of E-E bond or bonds (formation of dimers, oligomers or polymers) with concomitant releasing H_2. Titanium catalytic systems is generated by treatment of titanium(IV) complexes with different molar ratio of alkylating species. The predominant interest is focused on the role of ligand stability and the oxidation state of the active titanium center on the reactivity of proposed catalytic systems and properties of prepared polymers. [Refs. 23, 24]

International co-operations

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

Publications

Original papers

1. Blechta V., Schraml J.: Improved Pulse Sequences for Measurement of Small Long-Range Couplings Between Heteronuclei (29Si-13C) at Natural Abundance. Magn. Reson. Chem. 47(6), 511-514 (2009).
2. Blechta V., Schraml J.: SQ-SQ Experiment for Determination of Relative Signs of Small nJ(29Si,13C) Couplings in a Wide Variety of Silicon Compounds. Magn. Reson. Chem. 47(12), 1019-1023 (2009).
3. Cuřínová P., Stibor I., Budka J., Sýkora J., Lang K., Lhoták P.: Anion Recognition by Diureido-calix[4]arenes in the 1,3-Alternate Conformation. New J. Chem., 33(3), 612–619 (2009).
4. Hoffman H.E., Jirásková J., Cígler P., Šanda M., Schraml J., Konvalinka J.: Hydroxamic Acids as a Novel Family of Serine Racemase Inhibitors: Mechanistic Analysis Reveals Different Modes of Interaction with the Pyridoxal-5′-phosphate Cofactor. J. Med. Chem. 52(19), 6032-6041 (2009).
5. Karban J., Kroutil J., Buděšínský M., Sýkora J., Císařová I.: Ring-Opening Reactions of Aziridines Fused to a Conformationally Locked Tetrahydropyran Ring. E. J. Org. Chem. 2009(36), 6399-6404 (2009).
6. Lechner M.L., Fürpass K., Sýkora J., Fischer R.C., Albering J., Uhlig F.: Functionalized Tetrastannacyclobutanes, Part I. J. Organomet. Chem. 694(26), 4209-4215 (2009).

7. Pavela R., Sajfrtová M., Sovová H., Karban J., Bárnet M.: The Effects of Extracts Obtained by Supercritical Fluid Extraction and Traditional Extraction Techniques on Larvae Leptinotarsa decemlineata SAY. J. Essent. Oil Res. 21(4), 1-7 (2009).
8. Polívková K., Šimánová M., Budka J., Cuřínová P., Císařová I., Lhoták P.: Unexpected Behaviour of Monospirothiacalix[4]arene under Acidic Conditions. Tetrahedron Lett. 50(46), 6347-6350 (2009).
9. Pošta M., Čermák Jan, Vojtíšek P., Sýkora J., Císařová I.: Diphosphinoazine Rhodium(III) and Iridium(III) Octahedral Complexes. Inorg. Chim. Acta 362(1), 208-216 (2009).
10. Storch J., Sýkora J., Čermák Jan, Karban J., Císařová I., Růžička A.: Synthesis of Hexahelicene and 1-Methoxyhexahelicene via Cycloisomerization of Biphenylyl-Naphthalene Derivatives. J. Org. Chem. 74(8), 3090-3093 (2009).
11. Šabata S., Blechta V., Karban J., Pleska A., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. Polish J. Chem. 83(11), 1953–1958 (2009).
12. Červenková Šťastná L., Čermák Jan, Cuřínová P., Sýkora J.: Synthesis and Fluxional Behavior of New "Haevy Fluorous" Cyclopentadienes. J. Organomet. Chem., in press.
13. Hetflejš J., Šabata S., Podešva J., Kovářová J., Prokůpek L., Netopilík M., Spěváček J., Sýkora J.: Novel Stabilizers Acting Simultaneously as Molecular-Weight Regulators of Soluble Elastomeric Polyurethanes. Polym. Degrad. Stabil., submitted.
14. Karban J., Sýkora J., Kroutil J., Císařová I., Padělková Z., Buděšínský M.: Synthesis of All Configurational Isomers of 1,6-Anhydro-2,3,4-trideoxy-2,3-epimino-4-fluoro-β-D-hexopyranoses. J. Org. Chem., submitted.

Chapters in books

15. Blechta V.: Applications of Silicon-Carbon Coupling Constants. In: Annual Reports on NMR Spectroscopy. (Webb, G.A., Ed.), pp. 97-264, Elsevier, Amsterdam 2009.
16. Topka P., Zub Y.L., Karban J., Šolcová O.: Designing (Al-)SBA-15 Catalyst Pellet with Unique Properties. In: Characterisation of Porous Solids VIII. (Kaskel, S., Ed.), pp. 287-294, CRC Press, Cambridge 2009.

International conferences

17. Blechta V., Schraml J.: Small 29Si-13C Couplings and Their Signs for Any Spin System at Natural Abundance. 24th NMR Valtice, Sborník abstraktů, p. C-13, Valtice, Czech Republic, 26-29 April 2009.
18. Blechta V., Sýkora J., Kurfürst M., Sychrovský V., Schraml J.: 29Si- 13C Couplings across Two, Three, and Four Bonds in Alkoxy and Aryloxy Silanes. 5th European Silicon Days, Programme, Abstracts, and List of Partic., p. 189, Vienna, Austria, 20-22 September 2009.
19. Cuřínová P., Budka J., Budková M., Zajícová M., Pálková R., Sýkora J., Lhoták P., Stibor I.: Complexation Properties on the New Calix[4]Arene – Based Receptors. 24th NMR Valtice, Sborník abstraktů, p. C-35, Valtice, Czech Republic, 26-29 April 2009.
20. Kroutil J., Karban J.: Nucleophilic Ring Opening of Monosaccharide Aziridines. 15th European Carbohydrate Symposium Eurocarb 15, Book of Abstracts, p. 310 (PA 128), Vídeň, Austria, 19-24 July 2009.
21. Kurfürst M.: (LC-)29Si NMR Analysis of Silicon Oligomers. Magnetic Moments in Central Europe 2009, Book of Abstracts, p. P-15, Otocec, Slovenia, 11-15 February 2009.
22. Kurfürst M., Schraml J.: Structure Determination of Oligomeric Siloxanes. 24th NMR Valtice , Sborník abstraktů, p. C-22, Valtice, Czech Republic, 26-29 April 2009.
23. Pinkas J., Horáček M., Mach K., Gyepes R., Merna J., Sýkora J.: Dehydrogenative Polymerization of Phenylsilane Catalyzed by Titanium Complexes Effect of Ligand Framework on the Catalyst Reactivity. 41st Symposium on Catalysis, Program Book of Abstracts, p. 6, Prague, Czech Republic, 02-03 November 2009.
24. Pinkas J., Horáček M., Mach K., Gyepes R., Merna J., Sýkora J.: Titanium Complexes as Catalysts for Dehydrocoupling of Silanes. 3th Czech-Italian-Spanish Trilateral Meeting on Catalysis and Micro/Meso-Porous Materials (CIS-3), Book of Abstracts, p. O18, Acireale, Sicily, Italy, 21-25 June 2009.
25. Sajfrtová M., Karban J., Klouček P., Malík J., Kokoška L: Supercritical Fluid Fractionation for Thymoquinone Enrichment in Black Cumin and Savory Isolates. 57th International Congress and Annual Meeting of the Society for Medicinal Plant and Natural Product Research, Abstracts, Planta Medica 9(75), 1041, 2009, Geneva, Switzerland, 16-20 August 2009.
26. Sajfrtová M., Rochová K., Karban J., Sovová H., Pavela R.: Insecticide Activity of Peppermint and Lavender Extracts Isolated by Different Methods. 57th International Congress and Annual Meeting of the

Society for Medicinal Plant and Natural Product Research, Abstracts, Planta Medica 9(75), 1053, 2009, Geneva, Switzerland, 16-20 August 2009.

27. Sajfrtová M., Sovová H., Karban J., Pavela R.: Využití superkritické extrakce pro izolaci botanických insekticidů. (Czech) Utilization of Supercritical Fluid Extraction for Botanical Insecticide Isolation. 56. Konference chemického a procesního inženýrství CHISA 2009, Sborník, p. 143, Srní, Šumava, Czech Republic, 19-22 October 2009.
28. Sajfrtová M., Sovová H., Rochová K., Bártlová M., Wimmer Z.: Preparation of Extracts Rich in beta-Sitosterol Using Supercritical CO2. 2nd International Congress on Green Process Engineering, Proceedings, Venice, Italy, 14-17 June 2009.
29. Schraml J., Blechta V., Sýkora J., Kurfürst M., Sychrovský V.: 29Si-13C Couplings along the Si-O-C-C-C Chain in Aromatic and Aliphatic Compounds. Magnetic Resonance Conference EUROMAR 2009, Programme and Abstract Book, p. 94 (Sm14), Göteborg, Sweden, 05-09 July 2009.
30. Sýkora J., Storch J.: LC-NMR in Organic Synthesis of Hexahelicene Derivatives. Magnetic Moments in Central Europe, Program and Book of Abstracts, p. 93, Otočec, Slovenia, 11-15 February 2009.
31. Topka P., Karban J., Soukup K., Šolcová O.: Evaluation on Textural, Mechanical, and Catalytic Properties of Al-SBA-15 Pellets with Low Content of Silica Binder. 41st Symposium on Catalysis, Program Book of Abstracts, pp. 76-77, Prague, Czech Republic, 02-03 November 2009.
32. Topka P., Soukup K., Karban J., Šolcová O.: Catalytic Activity of Al-SBA-15 Pellets with Low Content of Additives in Friedel-Crafts Alkylation. 3rd International Symposium Advanced Micro- and Mesoporous Materials, Book of Abstracts, p. 140, Albena, Bulgaria, 06-09 September 2009.

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