

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 2006

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GENERAL INFORMATION

The Institute of Chemical Process Fundamentals (ICPF) is one of six institutes constituting the Section of Chemical Sciences of the Academy of Sciences of the Czech Republic. The Institute serves as a 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)	Eva Melková
Scientific Secretary	Jan Linek
Scientific Board Chairman	Karel Aim

DEPARTMENTS

Department of Separation Processes (page 5)
E. Hála Laboratory of Thermodynamics (page 16)
Department of Catalysis and Reaction Engineering (page 24)
Department of Multiphase Reactors (page 33)
Department of New Processes in Chemistry and Biotechnology (page 42)
Environmental Process Engineering Laboratory (page 49)
Laboratory of Aerosol Chemistry and Physics (page 55)
Laboratory of Laser Chemistry (page 62)
Department of Analytical Chemistry (page 67)

STAFF

(31 December 2006)

Category	Number of Employees
Research	132
Technical	20
Administrative	14
Services	18

BUDGET 2006

(23 Kč ≈ 1 US\$, 28 Kč ≈ 1 EUR)

Resources	Million Kč
Institutional support based on Institutional Research Plan	75
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	32
Foreign R&D Funds and European Programmes	4
Contracts with industry	2
Total Resources	113

Expenses	Per cent of Total Resources
Personal expenses including mandatory insurance	62
Purchase of material	11
Purchase of services	7
Repairs and maintenance	4
Depreciation of fixed assets	7
Travel expenses	4
Energy, water, and fuels	4
Total other expenses	1

Abbreviations used throughout the Report

ASCR	Academy of Sciences of the Czech Republic
GA ASCR	Grant Agency of the Academy of Sciences of the Czech Republic
GA CR	Grant Agency of the Czech Republic
ICPF	Institute of Chemical Process Fundamentals ASCR, Prague
ICT	Institute of Chemical Technology, Prague
CTU	Czech Technical University, Prague
CU	Charles University, Prague
TU	Technical University

Department of Separation Processes

Head: V. Jiříčný
Deputy: A. Heyberger
Research staff: J. Čermáková, J. Hanika, L. Hanková, L. Holub, P. Izák, K. Jeřábek,
J. Ondráček, R. Petříčkovič, M. Rousková, M. Sajfrtová, K. Setničková,
H. Sovová, P. Uchytíl, E. Volaufová
Part time: V. Staněk, H. Vychodilová
Technical staff: A. Kadlecová, D. Karfík, M. Koptová, D. Vlček
PhD students: K. Aleksieva, J. Křišťál, K. Rochová, P. Stavárek

Fields of research

- Hydrodynamic study of dynamic behaviour of two-phase co- and counter-current gas-liquid pulse flow in packed bed column
- Hydrodynamics of two phase flow in narrow channel
- Liquid extraction of tall oil from wastewaters of paper industry
- Supercritical fluid extraction of natural products; Enzymatic reactions in supercritical CO₂; Solubilities of liquids and solids in dense CO₂ with entrainer
- Relation between the morphology and application properties of polymer catalysts and adsorbents
- Study of the sorption in steady state of vapour permeation, model of toluene transport in polyethylene membrane during vapour permeation
- Conditions of vapour condensation in pores of Vycor, model of competitive adsorption on Vycor glass membrane

Applied research

- Research and development of three-dimensional electrodes in metal electrowinning and wastewater treatment
- Intensification and safety operation of trickle bed reactors under conditions of liquid phase pulse flow
- Extraction of polyaromatic hydrocarbons from aromatic petroleum fraction (300–400 °C)
- Refining of plant extracts
- Extraction and refining of plant extracts
- Supercritical fluid extraction of biologically active substances from plants
- Applications of ion exchangers as catalysts in various industrial processes

Research projects

Integrated multiscale process units with locally structured elements (IMPULSE)

(J. Hanika, V. Jiříčný, J. Drahoš, 6. 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. Another our activity consists in the implementation of numerical simulations for the prediction of two-phase flows in narrow channels. We also participate in the workpackage dealing with the results dissemination: "IMPULSE Workshop on integrated multiscale process units with locally structured elements" was organized in the frame of the international congress "CHISA2006". The results of this research are a part of the research in several subtasks of the project. [Refs. 45-49]

New procedures for an operation of industrial trickle bed reactors – intensification and safety control

(V. Jiříčný, joint project with ICT and Research Institute of Inorganic Chemistry, Ústí n. Labem, supported by the Ministry of Industry and Trade, grant TANDEM No. FT-TA/039)

Project is focused on the research and development of the know-how [Refs. 10, 36, 57, 58] and method of intensification [Refs. 24, 25, 37, 56] and safe control [Refs. 8, 35, 38] of industrial trickle bed reactors. The effect of liquid feed rate modulation and hydrodynamics of liquid pulse flow on conversion and selectivity of high-pressure hydrogenation process is studied [Refs. 42, 60-62].

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

(A. Heyberger, supported by AS CR, integration research project 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. 39, 53, 59]

Enzymatic catalysis in supercritical carbon dioxide

(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry of the ASCR, supported by Ministry of Education, COST project D30.001)

Enzymatic modifications of blackcurrant seed oil in supercritical carbon dioxide are studied in a continuous-flow reactor linked to an extractor filled with ground seeds [Refs. 20, 40]. The aim is to develop an integrated production and product recovery process for the extraction and lipase catalysis in supercritical CO₂. A study of canola oil hydrolysis [Ref. 9] is related to the project.

Enzymatic reaction in supercritical carbon dioxide: application to substances with pharmacological importance

(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry of the ASCR, supported by GA CR, grant No. 203/04/0120)

The project is focused on obtaining α - and γ -linolenic acids from blackcurrant seed *via* a new procedure where enzymatic hydrolysis or ethanolsis of blackcurrant oil [Ref. 54] follows after its supercritical fluid extraction from the seed [Ref. 51]. The aim of the project is to obtain variable and controlled α - to γ -linolenic acid ratios in different fractions of the reaction mixture. HPLC and other techniques are used to analyze the reaction products [Refs. 2, 50, 65]. As the applied enzyme, Lipozyme, is 1,3-specific, stereochemical distribution of fatty acids in vegetable oil is studied [Ref. 20].

Two challenges of supercritical fluid processes: flow pattern in extractor/reactor and fractionation of outflowing mixture

(H. Sovová, supported by GA CR, grant No. 104/06/1174)

Two aspects of supercritical processes are examined. First, tracer-response curves are measured in order to determine the axial dispersion in a continuous flow of supercritical solvent through packed bed of extracted particles or immobilized enzyme. Second, the effect of pressure and temperature on phase equilibrium in the mixtures of phytocomponents with CO₂ is measured in order to optimize the conditions for a partial separation of the mixture by its gradual expansion [Refs. 6, 22, 12-14, 43].

Supramolecular, natural phytosterol-based materials for applications in biology

(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry of the ASCR, ICT and Chemispol, supported by Ministry of Education, project No. 2B06024)

Phytosterols are extracted from plants with supercritical solvent using either pure carbon dioxide or, in the case of polar phytoecdysones, CO₂ modified with polar liquids. Different plants and different extraction conditions are examined in order to optimize the composition of extracts, which are used as substrates for synthesis of supramolecular materials.

Optimization of supercritical fluid extraction for maximum recovery of biologically active substances from plants

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

Biologically active substances are isolated from plants using different techniques as supercritical extraction [Refs. 21, 26], hydrodistillation [Ref. 11], Soxhlet extraction and maceration. The proper technique is chosen and operation conditions are optimized according to biological activity of the extracts against insect. A correlation between the composition of extracts and their biological activity will be derived.

Relations between morphology and activity of polymer-supported catalysts

(K. Jeřábek, supported by ICPF)

The project is connected with our long-time research of morphology of swollen functional polymers [Ref. 66]. A study was finished of differences in sensitivities of various reactions toward morphology of the polymer supports [Ref. 7]. In cooperation with Italian colleagues from Padua University, Italy, we studied the metal nanoparticle catalysts supported in polymer gel networks. [Refs. 15-17]

Polymer adsorbents additionally crosslinked using residual double bonds – synthesis, characterization and applications

(K. Jeřábek, supported by Ministry of Education, project no. 1P05ME740)

In cooperation with Chinese colleagues from the Nankai University, Tianjin, the effects were investigated of additional crosslinking of styrenic polymers using Friedel-Crafts

catalyzed reaction of double bonds remaining in the polymer after conventional polymerization. The morphology changes were examined by various techniques, including conventional nitrogen sorption porosimetry, inverse steric exclusion chromatography [Refs. 1, 27, 67], atomic force microscopy, and others.

Study of transport phenomena in polymeric membrane during pervaporation

(P. Uchytil, supported by GA ASCR, grant No. IAA4072402)

New type of the cell for the determination of transport parameters during vapor permeation through polymeric membranes was proposed and constructed. This apparatus makes possible performing permeation and steady state sorption experiments practically simultaneously. This novel experimental approach was tested in a study of propan-1-ol transport through a linear low-density polyethylene (LLDPE) membrane in a range of experimental conditions (membrane thickness, feed concentration, temperature) [Refs. 5, 30-32, 63]. We continued in the mathematical modelling, which includes the non-perfect step input concentration function, for the estimation of diffusion coefficient evaluation errors as dependence on the experimental arrangements and on the membrane transport properties [Ref. 3].

Ceramic materials with hierarchical porous structure for membrane separation technologies

(P. Uchytil, joint project with Institute of Chemical Technology, Prague, J. Heyrovský Institute of Physical Chemistry, supported by GA ASCR, grant No. 1QS401250509)

The transport and the separation efficiency in porous membranes are strongly influenced by the condensation of permeating substance. We proposed to use dynamic permeation method for studying the transport study of a condensable gas (butane) in porous microporous membranes [Refs. 29, 63]. The suggested experimental arrangement enables to measure the mass transport under changing pressure gradients in a membrane even for very small values of the pressure gradient across the membrane. In order to analyze the transient diffusion experiments a transport model was applied which is based on the Dusty Gas Model for the quantification of gas phase transport and on the generalized Stefan-Maxwell theory for the description of the transport of adsorbed species. The model describes relatively well exchange experiments performed with H₂ and N₂ or He and CO₂. It was found that the quality of the theoretical results for experiments with adsorbable gases depends strongly on the reliability of the model applied to quantify the adsorption isotherms [Refs. 32, 64]. The mathematical model for the mass transport through ceramic porous membranes was developed [Refs. 33, 44].

Flow of saturated vapor through porous membranes

(P. Uchytil, joint project with Technische Universität Wien, supported by Ministry of Education, KONTAKT project, No. 6-06-2)

The aim of the collaboration is an experimental investigation and an analysis of the flow of vapors through micro-porous membranes, under conditions where the Joule-Thomson effect has a large influence on the flow process. Specifically, the first aim is a systematic experimental study of the mass flow of different fluids through membranes with different pore sizes in the pressure range of permeant condensation.

International co-operations

ÅBO Akademi Process Chemistry Centre, Finland: By-product in the technology of sulfate cellulose production

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

Institut National Polytechnique de Lorraine, Nancy, France: Research of electroorganic synthesis in electrochemical micro reactor

Institute of Macromolecules, St. Petersburg, Russian Academy of Science, Russia: Separation of mixtures ethanol/toluene on cellulose myristate membrane

Institute für Mikrotechnik Mainz, Mainz, Germany: Research and development of micro devices

Otto von Guericke University of Magdeburg, Magdeburg, Germany: Influence of capillary condensation effects on mass transport through porous membranes

Solvent Innovation GMBH, Köln, Germany: Research of electroorganic synthesis in electrochemical micro reactor

Technical University, Bratislava, Slovakia: Polymer supported catalysts

Technical University of Crete, Chania, Greece: Research of composition and size of aerosols

Technische Universität Wien, Institut für Strömungslehre und Wärmeübertragung, Austria: Flow of saturated vapors through porous membranes

University of Barcelona, Barcelona, Spain: Morphology of polymer catalysts

University of California, Berkeley, USA: Research and development of three-dimensional electrodes

University of Linz, Linz, Austria: Determination of organic pollutants in water

University of Padua, Padua and University of L'Aquila, L'Aquila, Italy: Molecular accessibility of microporous matrixes

Nankai University, Tianjin, China: Hypercrosslinked polymer adsorbents

University of Skopje, Skopje, Macedonia: Extraction of hydroxycarboxylic acids; Supercritical fluid extraction of natural products

Visits abroad

A. Heyberger: CSIR of Johannesburg and Durban, Republic of South Africa (3 weeks)

P. Izák: University of Lisboa, Portugal, and University of Rostock, Germany (1 year)

J. Ondráček: Technical University of Crete, Chania, Greece (12 months)

Visitors

M. Čárský, University of Durban, Republic of South Africa

J. Dudas, CSIR, Johannesburg, Republic of South Africa

A. Siebalak, University of KwaZulu Natal, Durban, Republic of South Africa

T. Akramov, Bashkir University, Ufa, Russia

Teaching

H. Sovová: ICT, postgraduate course "Properties and application of supercritical fluids"

J. Hanika: ICT Prague, course "Multiphase Reactors"

J. Hanika: ICT Prague, course "Pharmaceutical Engineering"

J. Hanika: University Pardubice, course "Industrial Catalysis"

Publications

Original papers

1. Aleksieva K., Jing Xu., Wang Li min., Sassi A., Pientka Z., Zhang Z., Jeřábek K.: Effects of Post-Crosslinking of Macroreticular Styrene-Divinylbenzene Copolymers on Their Morphology. *Polymer* 47(19), 6544-6550 (2006).
2. Bártlová M., Bernášek P., Sýkora J., Sovová H.: HPLC in Reversed Phase Mode: Investigation of Kinetics of Blackcurrant Seed Oil Lipolysis in Supercritical Carbon Dioxide. *J. Chromatogr., B: Biomed. Appl.* 839(1-2), 80-84 (2006).
3. Čermáková J., Fialová K., Petříčkovič R., Kudrna V., Uchytíl P.: Influence of Non-Perfect Step Input Concentration at the Feed Side of the Membrane Surface on the Diffusion Coefficient Evaluation. *Macromol. Theor. Simul.* 15(3), 246-251 (2006).
4. Čermáková J., Scargiali F., Siyakatshana N., Kudrna V., Brucato A., Machoň V.: Axial Dispersion Model for Solid Flow in Liquid Suspension in System of Two Mixers in Total Recycle. *Chem. Eng. J.* 117(2), 101-107 (2006).
5. Fialová K., Petříčkovič R., Sharma M., Uchytíl P.: Steady State Sorption Measurement and the Transport Mechanism in Polymeric Membrane during Vapor Permeation. *J. Membr. Sci.* 275(1-2), 166-174 (2006).
6. Galushko A.A., Sovová H., Stateva R.P.: Solubility of Menthol in Pressurised Carbon Dioxide – Experimental Data and Thermodynamic Modelling. *Chem. Industry Chem. Eng. Q.* 12(3), 152-158 (2006).
7. Hanková L., Holub L., Jeřábek K.: Relation between Functionalization Degree and Activity of Strongly Acidic Polymer Supported Catalysts. *React. Funct. Polym.* 66(6), 592-598 (2006).
8. Kaštanek F., Hanika J.: Úloha chemického inženýrství ve zvyšování bezpečnosti chemických výrob. (Czech) The Role of Chemical Engineering in Enhancement of Chemical Process Safety. *Chem. Listy* 100(2), 150-155 (2006).
9. Moquin P.H.L., Temelli F., Sovová H., Saldaña M.D.A.: Kinetic Modeling of Glycerolysis – Hydrolysis of Canola Oil in Supercritical Carbon Dioxide Media Using Equilibrium Data. *J. Supercrit. Fluids* 37(3), 417-424 (2006).
10. Ondráček J., Stavárek P., Jiříčný V., Staněk V.: The Behavior of Counter-Current Packed Bed in the Proximity of the Flooding Point under Periodic Variations of Inlet Velocities. *Chem. Biochem. Eng. Q.* 20(2), 147-155 (2006).
11. Sovová H., Aleksovski S.: Mathematical Model for Hydrodistillation of Essential Oils. *Flavour Frag. J.* 21(6), 881-889 (2006).
12. Sovová H., Aleksovski S., Bocevska M., Stateva R.P.: Supercritical Fluid Extraction of Essential Oils - Results of Joint Research. *Chem. Industry Chem. Eng. Q.* 12(3), 168-174 (2006).
13. Aleksovski S., Sovová H.: Supercritical CO₂ Extraction of *Salvia officinalis* L. *J. Supercrit. Fluids*, in press.
14. Bocevska M., Sovová H.: Supercritical CO₂ Extraction of Essential Oil from Yarrow. *J. Supercrit. Fluids*, in press.
15. Bolfa C., Zoleo A., Sassi A.S., Maniero A.L., Pears D., Jeřábek K., Corain B.: Cross-linked Poly-Vinyl Polymers versus Polyureas as Designed Supports for Catalytically Active M0 Nanoclusters. Part I. Nanometer Scale Structure of the Polyurea Support EnCat™ 40. *J. Mol. Catal. A-Chem.*, in press.
16. D'Archivio A.A., Tauro L., Galantini L., Panatta A., Tettamanti E., Giammatteo M., Jeřábek K., Corain B.: Cross-Linked Poly-4-vinylpyridines as Useful Supports in Metal Catalysis: Micro- and Nanometer Scale Morphology. *J. Mol. Catal. A-Chem.*, *Mol. Catal. A-Chem.* 268, 176-184 (2007).
17. De Zan L., Gasparovičová D., Králík M., Centomo P., Carro M., Campestrini S., Jeřábek K., Corain B.: Nanoclustered Palladium(0) Supported on a Gel-Type Poly-acrylonitrile–N,N-dimethylacrylamide–ethylenedimethacrylate Resin: Nanostructural Aspects and Catalytic Behaviour. *J. Mol. Catal. A-Chem.*, in press.

18. Kudrna V., Jahoda M., Siyakatshana N., Čermáková J., Majířová H., Machoň V.: Various Applications of the Dispersion Model for Flow Systems with Danckwerts' Boundary Conditions. *Chem. Eng. Sci.*, in press.
19. Procházka J., Heyberger A., Volaufová E.: Effect of Diluents on Sulfuric Acid Extraction with Trialkylamine. *AIChE J.*, submitted.
20. Sovová H., Lísa M., Holčápek M.: Characterisation of Stereochemical Distribution of Fatty Acids in Vegetable Oils Based on HPLC Analysis of Triacylglycerols. *Anal. Biochem.*, submitted.
21. Sovová H., Opletal L., Bártlová M., Sajfrtová M., Křenková M.: Supercritical Fluid Extraction of Lignans from Caulomas and Leaves of *Schizandra chinensis*. *J. Supercrit. Fluids*, submitted.
22. Sovová H., Stateva R.P., Galushko A.A.: High Pressure Equilibrium of Menthol + CO₂. *J. Supercrit. Fluids*, in press.
23. Izák, M. Köckerling, U. Kragl; Stability and Selectivity of a Multiphase Membrane, Consisting of a Dimethylpolysiloxane on Ionic Liquid, Used in the Separation of Solutes from Aqueous Mixtures by Pervaporation, *Green Chem.*, 8 947-948 (2006).
24. Tukač V., Šimíčková M., Chyba V., Lederer J., Kolena J., Hanika J., Jiříčný V., Staněk V., Stavárek P.: The Behaviour of Pilot Trickle-Bed Reactor under Periodic Operation. *Chem. Eng. Sci.*, in press.
25. Hanika J., Jiříčný V., Kolena J., Lederer J., Staněk V., Tukač V.: Trickle Bed Reactor Operation under Forced Liquid Feed Rate Modulation, *Chem. Eng. Journal*, in press.

Chapters in books

26. Sovová H.: Modeling of Supercritical Fluid Extraction of Bioactives from Plant Materials. In: *Functional Foods Ingredients and Nutraceuticals*. (Shi, J., Ed.), pp. 76-109, CRC Press, New York 2006.

International conferences

27. Aleksieva K., Hanková L., Zhang Z., Jeřábek K.: Effects of Post-Crosslinking of Macroreticular Styrene-Divinylbenzene Copolymers of Their Morphology. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 65 (10 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
28. Břenková L., Bělohav Z., Durdil P., Eliášová H., Hanika J., Jašprová D., Tomášek V., Zámstný P.: Particles Segregation in Pharmaceutical Mixtures for Direct Tablets Compression. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, pp. 883-884 (8 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
29. Čermáková J., Markovic A., Uchytíl P., Seidel-Morgenstern A.: Binary Adsorption of Propane, Butane and Carbon Dioxide Mixtures in Vycor Glass. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 536, Praha, Czech Republic, 27-31 August 2006.
30. Fialová K., Petříčkovič R., Uchytíl P.: Transport Phenomena in Polyethylene Membrane. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 358, Praha, Czech Republic, 27-31 August 2006.
31. Fialová K., Petříčkovič R., Uchytíl P.: Semi Empirical Model of Toluene Transport in Polyethylene Membrane. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 359, Praha, Czech Republic, 27-31 August 2006.
32. Fialová K., Petříčkovič R., Uchytíl P.: New Apparatus for Determination of Steady State Sorption of Permeating Substance within Polymeric Membrane. 17th Annual Meeting of the North American Membrane Society NAMS 2006, Program Book, p. 143, Chicago, USA, 12-17 May 2006.
33. Fíla V., Zikánová A., Kotek V., Hrabánek P., Navara V., Toni F., Uchytíl P., Šolcová O., Bernauer B., Kočířik M.: A Relative Importance of Mass Transfer Resistance of Membrane

- Support in Composite Membranes of the Type Silicate-1- α -Alumina. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 286, Praha, Czech Republic, 27-31 August 2006.
34. Gogová Z., Fugasová M., Hanika J.: Experimental Study of Catalyzed Wet Oxidation of Ethanol in a Stirred Slurry Reactor. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 251 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
 35. Hanika J.: Stationary and Dynamic Trickle Beds. Summer School Reactors for the 21st Century, Book of Abstracts, Kuusamo, Finland, 04-07 June 2006.
 36. Hanika J.: Aplikovaný výzkum v Ústavu chemických procesů AV ČR. (Czech) Applied Research in Institute of Chemical Process Fundamentals AS CR. 15. Konference Chemické technologie . Materiály . Petrochemie . Polymery . Ropa . Legislativa . Prostředí . Bezpečnost . APROCHEM 2006, Sborník přednášek, p. 1155-1159, Milovy, Czech Republic, 24-27 April 2006.
 37. Hanika J., Jiříčný V., Kolena J., Lederer J., Staněk V., Tukač V.: Trickle Bed Reactor Operation under Forced Liquid Feed Rate Modulation. XVIIth International Conference on Chemical Reactors, Scientific Program, p. 21 (12 pp. full text on CD-ROM), Athens-Crete, Greece, 15-19 May 2006.
 38. Hanika J., Jiříčný V., Kolena J., Lederer J., Staněk V., Stavárek P., Tukač V.: Intensification, Safe Operation and Control of Industrial Trickle Bed Reactors. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 1, p. 69-70 (8 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
 39. Heyberger A., Rousková M., Tříska J., Volaufová E., Krtička M.: Liquid-Liquid Extraction of Tall Soap by Hexane. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 404-405 (8 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
 40. Hlavsová R., Wimmer Z., Sovová H., Zarevúcka M.: Blackcurrant Seeds (Waste By-Product) as a Source of Pharmacologically Important Polyunsaturated Fatty Acids. 7th European Meeting on Environmental Chemistry EMEC7, Book of Abstracts, p. 166, Brno, Czech Republic, 06-09 December 2006.
 41. Izák P., Crespo J., Kragl U.: Ionic Liquid Membranes for Selective Downstream Processing. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 147 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
 42. Jiříčný V., Stavárek P., Staněk V., Hanika J., Vychodilová H.: Hydrodynamics of Two Phase Pulse Flow in Packed Bed Apparatus. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 328 (9 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
 43. Kokoška L., Havlík J., Valterová I., Sovová H., Sajfrtová M., Maršík P.: Antibacterial Activity of *Nigella sativa* Seed Essential Oil and Effect of Different Extraction Methods on Content of Its Active Principle, Thymoquinone. 54th Annual Congress on Medicinal Plant Research, *Planta Medica* 72(11), 1008, 2006, Helsinki, Finland, 29 August - 02 September 2006.
 44. Kotek V., Zikánová A., Hrabánek P., Kovandová K., Brabec L., Kočířik M., Fíla V., Navara V., Lhotka M., Bernauer B., Šolcová O., Uchytíl P.: A Contribution of Mass Transport Resistance of Ceramic Supports to the Overall Mass Transport Resistance of Composite Membranes of the Type MFI -Alumina. 9th International Conference on Inorganic Membranes, α Zeolite- Program and Abstracts, Lillehammer, Norway, 25-29 June 2006.
 45. Křišťál J., Havlica J., Jiříčný V.: Visualization of Two-Phase Flow in Thin-Gap Microreactor. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 5, p. 1483 (4 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
 46. Křišťál J., Havlica J., Jiříčný V.: Optimization of Thin-Gap Reactor Geometry for One-Phase Flow Using CFD Simulations. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 5, p. 1802, Praha, Czech Republic, 27-31 August 2006.
 47. Křišťál J., Havlica J., Jiříčný V.: Two-Phase Pressure Drop in Thin-Gap Microreactor with Electrochemically Generated Bubbles. 9th International Conferences on Microreaction

- Technology IMRET 9, Book of Abstracts, p. 277-278, Potsdam/Berlin, Germany, 06-08 September 2006.
48. Křišťál J., Havlica J., Jiříčný V.: Electrochemical Microreactor Hydrodynamics. 4th European Summer School on Electrochemical Engineering, Poster Abstracts, p. 36, Palić, Serbia, 17-22 September 2006.
 49. Křišťál J., Havlica J., Jiříčný V.: Bubble Flow in Thin-Gap Channel: Experiments and Simulations. IMPULSE Scientific Workshop, Book of Abstracts, Tarragona, Spain, 06-07 July 2006.
 50. Lísá M., Holčapek M., Bernášek P., Sovová H.: HPLC/MS Characterization of Products of Black Currant Oil Enzymatic Hydrolysis. 24th Informal Meeting on Mass Spectrometry, Book of Abstracts, p. MoPo30, Ustron, Poland, 14-18 May 2006.
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 56. Staněk V., Hanika J., Jiříčný V., Tukač V., Stavárek P.: A Mathematical Model of Catalytic Hydrogenation Reactor under Periodic Variation of the Feed Rate. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 1, pp. 82-83 (7 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
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E. Hála Laboratory of Thermodynamics

Head: K. Aim
Deputy: M. Lísal
Research staff: M. Bendová, J. Linek, L. Morávková, J. Pavlíček, J. Slovák, L. Vlček,
Z. Wagner, I. Wichterle
Part time: A. Malijevský, I. Nezbeda, M. Předota
Technical staff: S. Bernatová, Š. Psutka
PhD students: A. Babič, J. Jirsák

Fields of research

- Experimental determination and modelling of phase equilibria in fluid 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 and mesoscale simulations of polymeric/nanoparticle systems
- Development of molecular theory of polar and associating compounds (and their mixtures)
- Development of equations of state based on molecular theory
- Hydrophobic interactions
- Percolation and nucleation
- Application of statistical–mechanical models to real fluids
- Thermodynamic modelling and processing of thermodynamic data

Applied research

- Computerized bibliography of vapour–liquid equilibrium data (annually updated)

Research projects

Description of thermodynamic behaviour of fluid systems at superambient conditions based on molecular models

(K. Aim, supported by GA ASCR, grant No. A4072301)

New measured data on phase equilibria in binary carbon dioxide + methanol, + ethanol, + 1-propanol, and + 2-propanol systems over extended ranges of temperatures and pressures were processed by both cubic and molecular-based equations of state. Excess volumes for the system octane + 1-chlorohexane were determined along four isotherms between 298.15 K and

328.15 K at pressures up to 40 MPa. Research continued on the applications of the perturbation theory and on the development of perturbed-type equations of state for real alkanols based on the molecular-level primitive model of association as well as on extending the approach to describe fluid phase equilibria in binary alkanol + carbon dioxide mixtures. [Refs. 15, 26-29]

Supercritical phase equilibria and p-V-T behaviour

(M. Bendová, supported by GA CR, grant No. 104/06/P066)

An apparatus for the determination of high-pressure phase equilibria has been modified in order to allow measurements for systems containing carbon dioxide and ionic liquids and is currently being tested. Liquid-liquid equilibria in binary systems of 1-ethyl-3-methylimidazolium ethylsulfate + heptane, + methylcyclohexane, and + toluene and of [bmim][PF₆] + 1-butanol have been determined by the volumetric method. Obtained results are now under verification by the direct analytical method. [Refs. 2, 3, 30, 31]

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

(J. Linek, supported by GA CR, grant No. 104/06/0656)

Excess volumes at atmospheric pressure were determined in the systems of cyclohexane + pentane, + hexane, + heptane, + octane, and + nonane at 298.15 K. Density, sound velocity, excess volume, and adiabatic and isothermal compressibility of the cyclohexane + nonane system was measured and calculated along four isotherms between 298.15 K and 328.15 K at pressures up to 40 MPa. Novel fitting procedure for calculating density and isothermal compressibility from the Tait equation was developed. Densities and sound velocities were also measured for the system MTBE + toluene at four temperatures and atmospheric pressure. Statistic and gnostic methods were applied to fit the incomplete data of excess volumes. In addition, the density of propiophenone (PrPON) below its melting temperature was estimated both from the PrPON density measurements at higher temperatures and from the correlation of excess volumes of (toluene + PrPON) determined at temperatures below the PrPON melting temperature. [Refs. 14, 37, 38, 49]

Molecular-level simulations of chemically-reacting fluids in nanoporous materials

(M. Lisal, supported by GA CR, grant No. 203/05/0725)

Behaviour of chemically reacting fluids in nanoporous materials has been studied by molecular simulations. Nanomaterial models of different levels of realism, ranging from simple nanopores or single carbon nanotubes to networked structures of pores or disordered random nanoporous media were considered. In particular, the effect of confinement on chemical equilibrium of NO dimerization in nanopores has been studied. A novel simulation methodology has been developed to predict polymer reaction equilibrium. [Refs. 7, 8, 16, 39]

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

(M. Lisal, 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 bulk and in confinement have been developed and tested. [Refs. 9-13, 17, 40-42]

General equations of state of fluids from molecular principles and their application to thermophysical properties of fluid mixtures

(I. Nezbeda, supported by GA ASCR, grant No. A4072303)

Types of intermolecular interactions primarily responsible for the structure and thermodynamic behaviour of polar and associated fluids were identified. Based on this notion, primitive models of water, ammonia, lower alkanols, acetone, and hydrogen sulfide were constructed. Second-order thermodynamic perturbation theory has been developed and applied to these models. New molecular-based equation of state for water has been derived and examined for capturing the anomalies in real water behaviour. Thermodynamics of water + methanol mixtures has been studied by molecular simulations for different levels of description of intermolecular interactions. [Refs. 5, 35, 36, 44, 46, 48]

Application of advanced simulation methods for studying the structure, physico-chemical properties, and preparation of composites and nanomaterials

(I. Nezbeda, supported by ASCR, project No. 1ET100720409)

The research has continued on the development of new methods for computer modelling of nanomaterials and materials with complex surface and/or bulk structure. In particular we have (i) performed simulations studying the behaviour of fluids in the vicinity of a large molecule, (ii) carried out simulations of the thermodynamic cycle based on a new method of direct simulation at constant entropy, (iii) realized the first practical application of the Gibbs ensemble parallel sampling method, and (iv) proposed and implemented a method for assessing the effect of different types of intermolecular interactions on the properties of pure water. [Refs. 6, 18, 20, 23, 33, 45, 47]

Phase and chemical equilibria in systems of liquids and gases

(I. Wichterle, supported by ICPF, project No. 2902)

Phase equilibria of a model system with transesterification reaction, namely the quaternary ethanol + propyl acetate \leftrightarrow propanol + ethyl acetate system, have been experimentally investigated. Vapour-liquid equilibria in binary and ternary systems of species with selected functional groups (tert-butyl, isopropyl, carbonyl, ether, and hydroxyl) have been measured. Algorithms for (i) reliable evaluation of temperature-independent parameters from vapour-liquid equilibria covering a temperature range and (ii) robust determination of interaction parameters in equation of state from high pressure vapour-liquid equilibrium data were developed. The bibliographic database of VLE data has been updated and published within the Landolt-Börnstein encyclopaedia series. [Refs. 1, 4, 19, 21, 22, 25, 50]

Research Centre: Behaviour of multiphase systems under superambient conditions (BEMUSAC)

(J. Drahoš, I. Wichterle, supported by FP5 RTD EU - NAS2 72074)

The Centre integrates physical chemistry and chemical engineering research with the aim to develop new super-ambient processes based on gas-liquid-solid contacting. It represents reorientation of R&D potential activities towards the advanced fields of multiphase systems under extreme conditions. The innovation is based on further intensification of all hitherto existing contacts and links of the Centre with academia and industry in Europe. The following research topics were studied by the guest postdoctoral fellows: (a) simulation study of the thermodynamic properties of water-methanol mixtures; (b) determination of vapour-liquid equilibrium and the solubility of impurities in industrial-grade liquid carbon dioxide; (c) the

flow over a backward-facing step by measuring the instantaneous wall shear rate in the channel spanwise centerline; (d) volumetric oxygen mass transfer coefficient in the bubble column using dynamic pressure-step method [see Department of Multiphase Reactors]. Besides, the following lines of research were pursued: (i) Gas-liquid equilibria were determined at sub- and supercritical conditions in carbon dioxide + alcohol systems and in the carbon dioxide + 1-chloropropane system [Refs. 29, 34]; (ii) Supercritical extraction of fine products from natural raw material was performed experimentally - equilibrium and transport data were determined. Results obtained were correlated by using a model proposed at ICPF [see Department of Separation Processes].

International co-operations

DICAMP, University of Trieste, Italy: Phase equilibria for supercritical fluid technology
Technical University of Vienna, Austria: Colloids and theory of fluids
Université de Paris-Sud, Orsay, France: Phase equilibria of complex fluid systems
University of Ontario Institute of Technology, Oshawa, ON, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids
U. S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA: Mesoscale and molecular simulations of complex systems
Universidad Rovira i Virgili, Tarragona, Spain: Molecular-based studies of chemically reacting systems in nanoporous materials
ITODYS, University of Paris VII, France: Vapour-liquid equilibrium bibliographic database; Phase equilibria in selected systems
Oak Ridge National Laboratory, Oak Ridge, TN, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems
University of Leipzig, Leipzig, Germany: Fluids at extreme conditions

Visits abroad

M. Lísal: University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)
M. Lísal: Universidad Rovira i Virgili, Tarragona, Spain (1 month)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

P. Camp, University of Edinburgh, UK
K. Fuchizaki, Department of Physics, Ehime University, Japan (1 month)
B. Rousseau, Université de Paris Sud, Orsay, France
F. R. Siperstein, Universidad Rovira i Virgili, Tarragona, Spain
A. Trokhymchuk, Institute of Condensed Matter Physics, Lviv, Ukraine
P. Ungerer, Institut Francais du Pétrole, Rueil-Malmaison, France

Teaching

- M. Lísal: J. E. Purkyně University, Ústí n. L., courses "Parallel programming", "Applications of Molecular Simulations", "Numerical mathematics I" and "Numerical mathematics II"
- I. Nezbeda: J. E. Purkyně University, Ústí n. L., courses "Molecular theory of matter" and "Statistical physics I"
- I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"
- I. Nezbeda, M. Předota: CU, course "Introduction to computer simulations in many particle 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. Barhala A., Dragoescu D., Teodorescu M., Wichterle I.: Isothermal Vapour-Liquid Equilibria in Binary Mixtures of 1,2-Dichloroethane and 1,1,1-Trichloroethane with Cyclopentanone at Temperatures from 298.15 to 313.15 K. *J. Chem. Thermodyn.* 38(5), 617-623 (2006).
2. Bendová M., Řehák K., Matouš J., Novák J.P.: Liquid-Liquid Equilibrium in Ternary Systems N,N-dimethylformamide + 2-methylpentane + Methanol and N,N-dimethylformamide + Methylcyclohexane + Methanol. *Fluid Phase Equilib.* 239(1), 16-25 (2006).
3. Bendová M., Wagner Z.: Liquid-Liquid Equilibrium in Binary System [bmim][PF₆] + 1-Butanol. *J. Chem. Eng. Data* 51(6), 2126-2131 (2006).
4. Bernatová S., Aim K., Wichterle I.: Isothermal Vapour-Liquid Equilibrium with Chemical Reaction in the Quaternary Water + Methanol + Acetic Acid + Methyl Acetate System, and in Five Binary Subsystems. *Fluid Phase Equilib.* 247(1-2), 96-101 (2006).
5. González-Salgado D., Nezbeda I.: Excess Properties of Aqueous Mixtures of Methanol: Simulation Versus Experiment. *Fluid Phase Equilib.* 240(2), 161-166 (2006).
6. Jedlovský P., Předota M., Nezbeda I.: Hydration of Apolar Solutes of Varying Size: a Systematic Study. *Mol. Phys.* 104(15), 2465-2476 (2006).
7. Lísal M., Brennan J.K., Smith W.R.: Mesoscale Simulation of Polymer Reaction Equilibrium: Combining Dissipative Particle Dynamics with Reaction Ensemble Monte Carlo. I. Polydispersed Polymer Systems. *J. Chem. Phys.* 125(16), 501-515 (2006).
8. Lísal M., Brennan J.K., Smith W.R.: Chemical Reaction Equilibrium in Nanoporous Materials: NO Dimerization Reaction in Carbon Slit Nanopores. *J. Chem. Phys.* 124(6), 1-14 (2006).
9. Lísal M., Nezbeda I., Ungerer P., Teuler J.-M., Rousseau B.: Low-Temperature Vapor-Liquid Equilibria from Parallelized Molecular Dynamics Simulations. Application to 1- and 2-Methylnaphthalene. *J. Phys. Chem. B* 110(24), 12083-12088 (2006).
10. Malijevský A.: Alternative Fundamental Measure Theory for Additive Hard Spheres Mixtures. *J. Chem. Phys.* 125(19), 1-5 (2006).
11. Malijevský A., Yuste S.B., Santos A.: How "Sticky" are Short-Range Square-Well Fluids. *J. Chem. Phys.* 125(7), 1-12 (2006).
12. Malijevský A., Santos A.: Structure of Penetrable-Rod Fluids: Exact Properties and Comparison between Monte Carlo Simulations and Two Analytic Theories. *J. Chem. Phys.* 124(7), 1-17 (2006).

13. Malijevský A., Sokolowski S., Zientarski T.: Structure and Phase Behavior of Widom-Rowlinson Model Calculated from a Nonuniform Ornstein-Zernike Equation. *J. Chem. Phys.* 125(11), 1-7 (2006).
14. Morávková L., Linek J.: Excess Molar Volumes of (Propiophenone + Toluene) and Estimated Density of Liquid Propiophenone below Its Melting Temperature. *J. Chem. Thermodyn.* 38(10), 1240-1244 (2006).
15. Morávková L., Wagner Z., Aim K., Linek J.: (P, V_m , T) Measurements of (Octane + 1-Chlorohexane) at Temperatures from 298.15 K to 328.15 K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.* 38(7), 861-870 (2006).
16. Smith W.R., Lísal M., Brennan J.K.: Effects of Confinement on Chemical Reaction Equilibrium in Nanoporous Materials. *Lect. Notes Comput. Sci.* 3984, 743-751 (2006).
17. Smith W.R., Lísal M., Nezbeda I.: Molecular-level Monte Carlo Simulation at Fixed Entropy. *Chemical Physics Letters* 426(4-6), 436-440 (2006).
18. Vega C., Abascal J.L.F., Nezbeda I.: Vapor-Liquid Equilibria from the Triple Point Up to the Critical Point for the New Generation of TIP4P-like Models: TIP4P/Ew, TIP4P/2005, and TIP4P/Ice. *J. Chem. Phys.* 125(3), 3-9 (2006).
19. Bernatová S., Aim K., Wichterle I.: Vapor-Liquid and Chemical Equilibria in the Ethanol + Acetic Acid System at 348.15 K. *J. Chem. Eng. Data* 52(1), 20-23 (2007).
20. Předota M., Cummings P.T., Wesolowski D.J.: Electric Double Layer at the Rutile (110) Surface. 3. Inhomogeneous Viscosity and Diffusivity Measurement by Computer Simulations. *J. Phys. Chem.* 111(7), 3071-3079 (2007).
21. Pavlíček J., Wichterle I.: Reliable Evaluation of Temperature Independent Parameters in Correlation of Vapour-Liquid Equilibrium Data. *Fluid Phase Equilib.*, submitted.
22. Wagner Z.: Robust Method of Determination of Interaction Parameters of Equation of State from High Pressure Vapour-liquid Equilibrium Data. *Fluid Phase Equilib.*, submitted.

Review papers

23. Nezbeda I., Kolafa J., Lísal M.: Molekulární simulace klasických tekutin. (in Czech) *Molecular Simulation of Classical Liquids. Československý časopis pro fyziku* 56(3), 148-151 (2006).

Books and monographs

24. Linek J.: Annual Report 2005. 68 pp., Institute of Chemical Process Fundamentals AS CR, Prague 2006.
25. Wichterle I., Linek J., Wagner Z., Fontaine J.-C., Sosnkowska-Kehiaian K., Kehiaian H.V.: Landolt-Börnstein IV/13A. Vapor-Liquid Equilibrium in Mixtures and Solutions. 540 pp., Springer, Berlin, 2007.

International conferences

26. Aim K., Babič A., Nezbeda I.: Equation-of-State Study Based on Comprehensive Phase Equilibrium Data for Carbon Dioxide + Lower Alkanol Systems at Superambient Conditions. 22nd European Symposium on Applied Thermodynamics ESAT 2006, Proceedings, pp. 153-156, Helsingor, Denmark, 28 June - 01 July 2006.
27. Aim K., Lísal M., Nezbeda I., Ungerer P., Teuler J.-M., Rousseau B.: Low Temperature Vapor-Liquid Equilibria from Parallelized Molecular Dynamics Simulation: Application to 1- and 2-Methylnaphthalene. 22nd European Symposium on Applied Thermodynamics ESAT 2006, Proceedings, pp. 321-324, Helsingor, Denmark, 28 June - 01 July 2006.
28. Aim K., Lísal M., Nezbeda I., Ungerer P., Teuler J.-M., Rousseau B.: Recent Advances in Molecular Simulation of Thermodynamic Behaviour of Fluid Systems. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, pp. 410-411, Praha, Czech Republic, 27-31 August 2006.

29. Babič A., Aim K.: Experimental Determination and Correlation of VLE for CO₂ + Alkanol Systems at Superambient Conditions. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, pp. 504-505, Praha, Czech Republic, 27-31 August 2006.
30. Bendová M.: Liquid-Liquid Equilibrium in Binary Mixtures of 1-Ethyl-3-methylimidazolium Ethylsulfate and Hydrocarbons. Distillation & Absorption 2006, Book of Abstracts, pp. 574-580, Londýn, Great Britain, 04-06 September 2006.
31. Bendová M., Wagner Z.: Liquid-Liquid Equilibrium in Binary System [bmim][PF₆] + 1-Butanol. Experimental Data and Their Thermodynamic Description. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 507 (12 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
32. Eleftheriadis K., Vratolis S., Housiadas C., Smolík J., Ždímal V., Schwarz J., Wagner Z., Lazaridis M., Ondráček J., Hussein T., Kephelopoulos S., Drossinos Y.: Modal Structure of the Fine Urban Aerosol in four European Cities. 7th International Aerosol Conference, Proceedings, p. 1786, St. Paul, Minnesota, USA, 10-15 September 2006.
33. Gonzáles-Salgado D., Nezbeda I.: VLE Simulations of 1-Methyl-naphtalene with Explicit Interface. 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11-16 June 2006.
34. Chorazewski M., Babič A., Wichterle I.: Measurement of Vapour-Liquid Equilibrium at High Pressures and in Critical Region for Carbon Dioxide + 1-Chloropropane System. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 506, Praha, Czech Republic, 27-31 August 2006.
35. Jirsák J., Nezbeda I.: Molecular Mechanisms Underlying the Thermodynamic Properties of Water. 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11-16 June 2006.
36. Jirsák J., Nezbeda I.: Molecular-based Equation of State for TIP4P Water. EMLG 2006, Book of Abstracts, Barcelona, Spain, 03-07 September 2006.
37. Linek J., Morávková L.: Excess Volumes of (Propiophenone + Toluene) and Density of Liquid Propiophenone below Its Melting Temperature. 22nd European Symposium of Applied Thermodynamics ESAT 2006, Proceedings, pp. 401-404, Elsinore, Denmark, 28 June - 01 July 2006.
38. Linek J., Morávková L.: (P, V_m, T, x) Behaviour of the Toluene-Propiophenone Liquid Mixtures. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 70 (7 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
39. Lísal M.: Molecular-Level Monte Carlo Simulation at Fixed Entropy. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 288 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
40. Malijevský A., Bravo S.Y., Santos A.: High-Temperature and Low-Temperature Approximations for Penetrable-Sphere Fluids: Comparison with Monte Carlo Simulations. 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11-16 June 2006.
41. Malijevský A., Bravo S.Y., Santos A.: How "Sticky" are Short-Range Square-Well Fluids? 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11-16 June 2006.
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44. Moučka F., Nezbeda I.: A Quantitative Characterization of Structural Changes in the Hard-Disk Fluid near Freezing/Melting Conditions. 7th Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11-16 June 2006.

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Fields of research

- Catalytic combustion of volatile organic compounds in waste gases
- Transport processes in porous solids
- Sulphide catalysts of unconventional composition
- Unconventional preparation of supported molybdenum catalysts
- Texture of porous solids
- Design of new theoretical models for structure-activity relationships
- Theoretical analysis of the structure of molecules with complicated bonding pattern
- Temperature programmed techniques in characterization of catalysts

Applied research

- Catalytic combustion of volatile organic compounds
- Textural characteristics of structural materials
- Precipitation of ammonium aluminum alum by ammonia

Research projects

Nanostructured materials - texture from physical adsorption

(O. Šolcová, supported by GA CR, grant No. 104/04/0963)

Project develops and improves the methods for obtaining textural characteristics (e.g. pore-size distribution-PSD, t-plot) of porous materials from experimental physical adsorption isotherms of various gases. The up-to date evaluation methods have been applied together with newly obtained information on adsorbed film thickness. The novel hierarchic titania nanomaterials have been prepared. The obtained results are mutually correlated with pore structures established by high-resolution electron microscopy. [Refs. 7-8, 18, 22, 24, 28, 40-45, 60]

Diffusion coefficients and other transport characteristics of specially shaped porous supports and catalysts

(O. Šolcová, supported by GA ASCR, grant No. IAA4072404)

The project develops and verifies a new method for the determination of diffusion coefficients and other transport characteristics of industrial porous solids with non-standard shapes (which guarantee high outer surface to volume ratio). The chromatographic method in SPSC arrangement has been applied. To decrease the number of fitted parameters, the axial dispersion parameter (Peclet number) has been obtained independently of responses of SPSC packed with porous pellets with pores blocked by a suitable liquid - Porofil (nonporous packing). The obtained diffusion coefficients and other transport characteristics have been compared with characteristics from standard textural analyses. [Refs. 15, 17, 19-20, 58-59, 61]

Porous catalysts and membrane supports: a relationship between mass transport and textural properties

(V. Hejtmánek, supported by GA CR, grant No. 203/05/0347)

The objective of this project is a modern approach to characterization of catalyst and membrane support pore structures and the investigation of a relationship between mass transport and pore structure. The pore structure characterization (reconstruction of pore space) of macroporous solids is namely accomplished by the generation of 3D image from many serial 2D cuts of actual porous media. The reconstructed pore space serves as the key information for the development of a 3D random pore network model, which allows study of a more rational prediction of mass transport phenomena in porous solids. The application of the project results in heterogeneous catalysis, separation processes, and development of new catalysts is of primary interest. [Refs. 7, 17, 33-34]

Organised materials for highly selective catalytic and separation processes

(K. Jiráťová, supported by GA CR, grant No. 203/03/H140)

Wide research group involving mostly PhD students is mainly oriented on the cooperation among them and gaining of the co-applicant's know-how in the research areas covering the topic of the proposal. Scientific aim of the project comprises synthesis of catalytic and separation structures by methods of nanotechnologies and nanoengineering. The structural and functional characterization of the prepared materials and of the process modeling is of primary importance. The obtained results have been presented in a number of contributions in scientific journals and international symposia. [Refs. 18-19, 22-23, 28, 41-50, 58-60]

Study of factors influencing the activity and selectivity of supported bimetallic transition metal sulfides in HDS and HDN reactions

(Z. Vít, supported by GA CR, grant No. 104/06/0870)

This project concerns basic research of the preparation of supported noble metal sulfides selected from Rh, Ru, Pd or Pt in combination with Mo sulfide and study of their catalytic behaviour mainly in HDS and HDN. The Pt based catalysts exhibited interesting hydrogenation activity; pyridine was consumed more easily than thiophene. The acidity of supports plays a positive role in the HDN, which has also been documented by us in the case of Mo promoted by Rh. The deposition of the Pt-Mo combination on acidic support like silica-alumina will further lead to enhanced HDN activity and HDN/HDS selectivity. [Refs. 20, 32]

Synergistic effects in hydrodesulfurization and oxidation reactions

(K. JirátoVá, bilateral co-operation with Institute of Catalysis, Sofia, Bulgaria)

Temperature programmed techniques were used to characterize physical-chemical properties of the FeMoP/TiO₂ and NiW/alumina catalysts of various Fe/Mo and Ni/W molar ratio and the effect of catalytic support. [Refs. 10, 12]

Influence of chemical and phase composition of hydrotalcite based material on the catalytic activity for nitrous oxide decomposition

(K. JirátoVá, supported by GA CR, grant No. 106/05/0366)

The calcined Co(Mg)Mn(Al) hydrotalcite-like compounds are active even in decomposition of nitrous oxide. Properties and catalytic activity of the catalysts having various molar ratios of Co:Mg:Mn:Al, the structure-activity relationship in this reaction carried out over Ni-(Mg)-Al and Ni-(Mg)-Mn systems, and the effect of Ni-Al crystallinity were examined. The Co₄MnAl catalyst is the most active. The influence of inlet composition (presence of CO) was examined in detail. [Refs. 9, 11, 51-54]

New catalytic materials for combustion of VOC and their properties

(K. JirátoVá, supported by GA CR, grant No. 104/04/2116)

Properties of calcined Co(Mg)Mn(Al) hydrotalcite-like compounds are examined and their activity in combustion of model VOC as well. We found that the activity of the calcined catalysts increases with the amount of compounds (Co³⁺ and Mn⁴⁺). All catalysts with the highest activity showed low values of basicity at the same time. The effect of LDH precursor crystallinity was studied over the Ni₄Al₂ system. The highest catalytic activity was found with the system having not too high crystallinity. [Refs. 9, 23, 26, 46-50]

Catalysis over sulfides: preparation of catalysts by solvent assisted spreading and the effect of support type on synergistic effect

(M. Zdražil, supported by GA ASCR, grant No. IAA4072306)

MoO₃/MgO catalysts were prepared by the reaction of MgO extrudates (diameter 1.6 mm, S_{BET}=311 m² g⁻¹) with the MoO₃/methanol slurry at room temperature. Sharp and deep eggshell Mo concentration profiles were formed. With sufficient MoO₃ amount, the shell thickness increased with time until support saturation. Planetary mill ground MoO₃ reacted much faster than MoO₃ ground in an agate mortar mill. Uniform saturated loading of 19% was achieved after 5 days in the former case while 11 days was not sufficient for support saturation in the latter case. Hydrodesulfurization activity of saturated MoO₃/MgO catalyst was the same as of commercial MoO₃/Al₂O₃. [Refs. 5, 31]

Unconventional supports in catalysis over sulfides

(M. Zdražil, supported by GA CR, grant No. 104/06/0705)

MoO₃/TiO₂ catalysts were prepared by reaction of TiO₂ extrudates (140 m² g⁻¹) with a MoO₃/H₂O slurry. The adsorption of molybdena species was strong; sharp and deep eggshell profiles of the Mo concentration were obtained. The hydrodesulfurization activity of saturated catalysts with a uniform Mo distribution (about 10 mass % MoO₃) was at least the same as that of a sample prepared by conventional impregnation. [Ref. 6]

Preparation of supported catalysts by slurry impregnation

(L. Kaluža, supported by GA CR, grant No. 104/06/P034)

Solvent assisted spreading of CoO over monolayer MoO₃/Al₂O₃ catalysts has been studied. CoCO₃.Co(OH)₂ and CoCO₃ reacted with MoO₃/Al₂O₃ in water slurries. CoO

deposition over $\text{MoO}_3/\text{Al}_2\text{O}_3$ extrudates was followed by EPMA. In the set of eleven $\text{MoO}_3/\text{Al}_2\text{O}_3$ catalysts, the amount of CoO adsorbed was roughly proportional to the surface area of MoO_3 monolayer. The adsorbed Co species efficiently enhanced the hydrodesulfurization activity. Moreover, MoO_3 and $\text{CoCO}_3 \cdot \text{Co}(\text{OH})_2$ deposition onto $\alpha\text{-AlOOH}$ during paste processing have been investigated as a method of choice to synthesise bimetallic $\text{CoMo}/\gamma\text{-Al}_2\text{O}_3$ catalysts for hydrodesulfurization. [Refs. 21, 36-39]

Role of electron pairing in chemical bonds

(R. Ponec, supported by GA ASCR, grant No. IAA4072403)

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, 3-center 4-electron bonding, hypervalence, etc. and to the quantitative characterization of the extended cyclic delocalization in aromatic hydrocarbons. [Refs. 1-3, 13, 16, 25, 29, 55-57]

Molecular basis of structure-activity relationships

(R. Ponec, Joint project with the University of Girona)

The project is a part of long-term collaboration with the Institute of Computational Chemistry of the University of Girona. The interest in this project is primarily focused on the design of new simple theoretical models and procedures allowing us to build up the microscopic basis both for traditional structure-activity relations as well as for the design of new theoretical QSAR models. [Ref. 4]

International co-operations

University of Liverpool, Liverpool, Great Britain: Analysis of the pair density matrix

University of Marburg, Marburg, Germany: Structure of complex inorganic molecules

University of California, Davis, USA: Multicentre bonding in organic chemistry

Institute of Computation Chemistry, University of Girona, Spain: Analysis of the pair density matrix, theory of structure-activity relationships

University of Ghent, Ghent, Belgium: Generalized population analysis, theoretical characterization of aromaticity

Institute of Catalysis, Sofia, Bulgaria: Synergistic effects in hydrodesulfurization and oxidation reactions

National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan: Promotion of Mo sulfide catalysts by dispersed noble metals

Höganäs AB, Höganäs, Sweden: Transport processes in the powdery metallurgy

Visitors

P. Bultinck, University of Ghent, Belgium
J. Chaves, University of Girona, Spain
J. Cioslowski, University of Szczecin, Poland
Y.L. Zub, Institute of Surface Chemistry NAS, Ukraine
M. Ludwik, Central Mining Institute, Poland

Teaching

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

Publications

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61. Šolcová O., Šnajdaufová H., Součková H., Schneider P.: Distribution of Through Pore- Sizes from Liquid Expulsion Permporometry. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 79 (11 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.

Department of Multiphase Reactors

Head: J. Drahoš
Deputy: J. Tihon
Research staff: M. Fialová, M. Fugasová, J. Havlica, S. Orvalho, M. Růžička, J. Slezák, V. Sobolík, V. Tovchigrechko, J. Vejražka, M. Večeř, O. Wein
Part time: V. Pěnkavová, M. Plzánková
Technical staff: S. Nováková
PhD students: R. Bunganič, Z. Gogová, L. Kulaviak, P. Stanovský, M. Šimčík

Fields of research

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

Research projects

Multi-scale hydrodynamics of gas-liquid reactors

(M. Růžička, joint project with TU Ostrava, supported by GA CR, grant No. 104/04/0827)

The project is focused on the basic research in the hydrodynamic interactions between the phases in gas-liquid reactors and contactors. The basic idea of the project is to decompose the hydrodynamic processes according to their length and time scales, to understand them separately and then to develop a synthetic model for the behaviour of the whole bubbly layer. The research approach combines experimental activity, theoretical modelling, and CFD. The project goal is to find the link between microscale and macroscale. [Refs. 1, 16, 18, 28, 29, 32-34, 38, 40, 42, 43, 46-51, 59]

Dynamics of direction-specific friction probes for electrodiffusion diagnostics of flow in rheologically complex liquids

(O. Wein, joint project with Institute of Hydrodynamics of the ASCR, supported by GA CR, grant No. 104/04/0826)

Electrodiffusion (ED) sensors work on the polarographic principle. With known depolarizer content in the liquid, the ED friction probe detects shear rate at its surface. Multi-segment ED friction probes, in addition, monitor also the varying flow direction. Unfortunately, their safe use is still limited to slowly varying flows. The computer-aided calibration and control of multi-segment ED probes would be improved by (i) including the effect of insulating gaps on dynamics (essential in fast changing flows), (ii) including the effect of longitudinal diffusion (essential in slow flows, low Peclet numbers), (iii) including the dynamic (voltage-step) direction-specific calibration on the individual segments, and incorporated into a new issue of the software EDWORK. For confirmation of the theory and algorithms, experiments in a well-controlled pulsating viscometric flow will cover a variety of

biological and polymeric liquids. The related data on diffusivities and viscosities would be an important by-product of the intended research. [Refs. 4, 5, 9, 10, 56-58]

Diagnostics of the near-wall turbulence in backward-facing step flows

(J. Tihon, supported by GA CR, grant No. 101/04/0745)

An experimental study of the near-wall turbulence in the backward-facing step flow is carried out with the aim to cover a wide range of operating parameters (the expansion ratio, the Reynolds number, inlet flow conditions). The electrodiffusion technique is applied to map the wall shear rate and to measure local mass transfer coefficients at the wall. The application of directionally sensitive, multi-segment sensors enables us to determine precisely the position of reattachment and to assess the effect of operation parameters on the size of recirculation zones and the strength of reverse flow close to the wall. These complex measurements provide new information about the behaviour of coherent flow structures in the near-wall region. [Refs. 6, 36, 37]

Hydrodynamic interactions of bubbles and particles in flotation process

(M. Růžička, joint project with ICT, supported by GA CR, grant No. 104/05/2566)

The goal of this project is the investigation of the interactions between solids and bubbles in the flotation process. Our activity is focused on the underlying physical mechanisms that control the basic steps of the interactions, namely the collision dynamics of bubbles with solids of comparable size, and the hydrodynamic and surface phenomena playing roles in the agglomerate formation and its stability. The project is designed to comprise a well-balanced composition of experimental, theoretical and CFD activities. The basic experimental tool is a sophisticated and advanced visualization technique based on digital high-speed imaging. The measured data will form a basis for theoretical considerations. The modeling concepts will be tested with CFD simulations and validated with the data. The main output will be a new concept for describing the interactions between bubbles and solids. [Refs. 1, 2, 16, 18, 20, 21, 23, 25, 26, 40, 41, 44, 53, 59]

Continual fermentation of non-alcoholic beer

(M. Růžička, joint project with ICT, supported by GA CR, grant No. 104/06/1418)

The goal of this project is the investigation of the rheological properties and hydrodynamic behaviour of a bed of carrier particles for supporting biomass in a gas-liquid-solid three-phase system. The particles are the spent grains, because of availability and low price. They form a bed ('sludge blanket') in the fermentor that tend to sediment and settle at the bottom. The fermentor is flown through the liquid phase with a recycle, to keep the bed in a quasi-fluidized state, which is required for the fermentation purpose. Occasionally, it is also sparger with gas, for technological reasons. Our goal is to find the values of control parameters when the bed neither settle nor escape from the reactor. [Refs. 1, 18, 28, 29, 40, 44]

Collision dynamics of bubbles and solid particles in liquids

(J. Havlica, supported by GA CR, grant No. 104/05/P554)

The project is aimed at one specific and well defined problem from three-phase hydrodynamics: interactions between a rising bubble and a moving solid particle in a liquid. The project includes three subsequent activities: (i) preparation of experimental apparatus and developing a device for production of bubbles of desired properties, (ii) experimental study of behavior of collision of a bubble and solid particle, (iii) suggestion of a theoretical model based on the results of the measurements and comparison of these results with CFD simulations. [Refs. 10, 20, 21, 25, 26, 57, 58]

Study of the bubble growth during boiling

(J. Vejražka, supported by GA CR, grant No. 101/05/P229)

Objective of the project is to explain processes taking place in detachment of the vapour bubble from a heated surface during boiling. The detachment is studied experimentally for both the vapour bubble and an air bubble injected through a needle. In the latter case, the needle can be rapidly moved in order to study different forces acting on the bubble. The results are compared with results of theoretical models. The main outcome will be the basis for building new models for predictions of heat transfer in nucleate boiling. [Refs. 7, 23, 42-44, 52-55]

Effect of bubble size on the stability of uniform bubble bed

(M. Večeř, supported by GA CR, grant No. 104/06/P287)

The goal of the project is to investigate experimentally the effect of the size of bubbles on the stability of the homogeneous flow regime in bubble column reactors, and its transition to the heterogeneous flow regime. The former regime lack large-scale motions of the two-phase mixture in the column, while convective currents ('circulations') set in, when loses the stability. There is a theoretical concept developed of the regime transition that is to be verified by measurements. This forms the core of this project. [Refs. 10, 14, 32, 38, 40, 46, 48-51, 57-59]

Reaction and transport phenomena in complex homogeneous and heterogeneous systems

(J. Drahoš, joint project with ICT, supported by GA CR, grant No. 104/03/H141)

The project is aimed at the preparation of PhD students for research and production activities in modern areas of chemical, pharmaceutical, biological and process industries. It includes both theoretical and experimental work of 20 students/year of ICT and ICPF in research programs directed to studies of hydrodynamics and transport processes in multiphase tower, stirred and membrane mass exchange systems, homogeneous and heterogeneous reactors and microreactors and to the studies of effects of electric field on chemical and biological systems. [Refs. 27, 41, 42, 44, 46-48, 51-53, 55]

Chairmanship of the EFCE working party on multiphase fluid flow

(J. Drahoš, INGO project supported by the Ministry of Education, LA 178)

The project supports networking activities and integration of members of the Department into the relevant scientific bodies at European level, like European Federation of Chemical Engineering (two members act as the respective chairman and secretary to the Working Party on Multiphase Fluid Flow) or European Multiphase Science Institute (one member was confirmed as the coordinator of one of totally six integration programmes of EMSI).

Research Centre: Behaviour of multiphase systems under superambient conditions

(J. Drahoš, I. Wichterle, supported by FP5 RTD EU - NAS2 72074)

The Centre integrates physical chemistry and chemical engineering research with the aim to develop new super-ambient processes based on gas-liquid-solid contacting. It represents reorientation of R&D potential activities towards the advanced fields of multiphase systems under extreme conditions. The innovation is based on further intensification of all hitherto existing contacts and links of the Centre with academia and industry in Europe. The following research topics were studied by the guest postdoctoral fellows: (a) simulation study of the thermodynamic properties of water-methanol mixtures; (b) determination of vapour-liquid equilibrium and the solubility of impurities in industrial-grade liquid carbon dioxide; (c) the flow over a backward-facing step by measuring the instantaneous wall shear rate in the

channel spanwise centerline; (d) volumetric oxygen mass transfer coefficient in the bubble column using dynamic pressure-step method [Refs. 17, 19, 20, 21, 26, 34, 40, 42, 44-46, 48, 51, 55]. Besides, the following lines of research were pursued: (i) Gas-liquid equilibria were determined at sub- and supercritical conditions in carbon dioxide + alcohol systems [see E. Hála Laboratory of Thermodynamics] and in the carbon dioxide + 1-chloropropane system; (ii) Supercritical extraction of fine products from natural raw material was performed experimentally – equilibrium and transport data were determined. Results obtained were correlated by using a model proposed at ICPF [see Department of Separation Processes].

Integrated multiscale process units with locally structured elements (IMPULSE)

(J. Hanika, V. Jiříčný, J. Drahoš, 6. 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 of electrodiffusion sensors for the experimental flow diagnostics in microreactors. Another our activity consists in the implementation of numerical simulations for the prediction of two-phase flows in narrow channels. We also participate in the workpackage dealing with the results dissemination: "IMPULSE Workshop on integrated multiscale process units with locally structured elements" was organized in the frame of the international congress "CHISA 2006" [See Department of Separation Processes].

Study of gas holdup non-uniformity in free bubble rise aerated vessels – extension of previous analysis

(M. Fialová, bilateral co-operation with Institute of Chemical Engineering, Sofia, Bulgaria)

Local gas hold-up distribution profiles in bubble column were compared with model solutions and the flow field variation obtained from CFD modeling was demonstrated. The effect of gas distributor on the characteristic of the gas dispersion within the bubble column was tested. [Refs. 19, 45]

International co-operations

CRTT, Saint Nazaire, France: Backward-facing step flows, Microfluidics

LEGI / IMG, Grenoble, France: Bubble columns

Institute of Fluid Mechanics, Toulouse, France: Hydrodynamic interactions of bubbles

Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow

Rovira i Virgili University, Tarragona, Spain: Impinging jets

University of Thessaly, Volos, Greece: Liquid film flows

Aristotle University, Thessaloniki, Greece: Electrodiffusion diagnostics of the flow

University of Minho, Braga, Portugal: Multiphase bubble bed reactors

University of Porto, Portugal: Hydrodynamics of g-l-s systems

Slovak Technical University, Bratislava, Slovakia: Mass transfer in bubble columns

Institute of Chemical Engineering, BAS, Sofia, Bulgaria: Gas-liquid reactors

Institute of Thermophysics, RAS, Russia: Diagnostics of multiphase flows

Twente University, Twente, The Netherlands: Hydrodynamics of bubbly flow

Worcester Polytechnic Institute, Worcester, USA: CFD

Technology Institute, SINTEF, Trondheim, Norway: Bubble columns
Kyoto University, Japan: Hydrodynamics of bubbly flow
Kobe University, Japan: Hydrodynamics of bubbly flow
Kyushu University, Fukuoka, Japan: Hydrodynamics of bubbly flow

Visits abroad

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

Visitors

S. Orvalho, Technical University of Lisbon, Portugal (8 months)
M. Pantzali, Aristotle University, Thessaloniki, Greece
N. Kazakis, Aristotle University, Thessaloniki, Greece
J. Comiti, University of Nantes, France
L. Uby, ITT Flygt, Sweden
V. Bontozoglou, University of Thessaly, Volos, Greece
T. Sanada, Kyushu University, Fukuoka, Japan
M. Watanabe, Kyushu University, Fukuoka, Japan
V. Báleš, Slovak Technical University, Bratislava, Slovakia

Teaching

J. Drahoš: ICT, postgraduate course "Multiphase reactors"
M. Růžička: ICT, course "Fluid Mechanics" and postgraduate course "Multiphase reactors"
J. Tihon: ICT, postgraduate course "Drops, bubbles and particles"
O. Wein: TU Brno, course "Principles of Rheology"
M. Večeř: TU Ostrava, course "Reactor Engineering"

Publications

Original papers

1. Hladil J., Růžička M., Koptíková L.: Stromatactis Cavities in Sediments and the Role of Coarse-Grained Accessories. *Bull. Geosci.* 81(2), 123-146 (2006).
2. Růžička M.: On Buoyancy in Dispersion. *Chem. Eng. Sci.* 61(8), 2437-3446 (2006).
3. Tihon J., Serifi K., Argyriadi K., Bontozoglou V.: Solitary Waves on Inclined Films: Their Characteristics and the Effect on Wall Shear Stress. *Exp. Fluids* 41(1), 79-89 (2006).
4. Wein O., Tovčigrečko V., Sobolík V.: Transient Convective Diffusion to a Circular Sink at Finite Peclet Number. *Int. J. Heat Mass Transfer* 49(23-24), 4596-4607 (2006).
5. Wein O., Večeř M., Tovčigrečko V.: AWS Rotational Viscometry of Polysaccharide Solutions Using a Novel KK Sensor. *J. Non-Newtonian Fluid Mech.* 139(1-2), 135-152 (2006).

6. Huchet F., Comiti J., Tihon J., Montillet A., Legentilhomme P.: Electrodifusion Diagnostics of the Flow and Mass Transfer inside a Network of Crossing Minichannels. (Eng) *J. Appl. Electrochem.* 37(1), 49-55 (2007).
7. Vejrazka J., Marty Ph.: An Alternative Technique for the Interpretation of Temperature Measurements Using Thermochromic Liquid Crystals. *Heat Transfer Eng.* 28(2), 154-162 (2007)
8. Fujasová M., Linek V., Moucha T.: Mass Transfer Correlations for Multiple-Impeller Gas-Liquid Contactors. Analysis of the Effect of a Axial Dispersion in Gas and Liquid Phase on "Local" kLa Values Measured by the Dynamic Pressure Method in Individual Stages of the Vessel. *Chem. Eng. Sci.*, in press.
9. Sobolík V., Wein O.: The Levich Problem with an Eccentric Segmented Electrode. *Russ. J. Electrochem.*, submitted.
10. Wein O., Večeř M., Havlica J.: End Effects in Rotational Viscometry I. No-Slip Shear-Thinning Samples in the Z40 DIN Sensor. *Rheol. Acta*, submitted.

Patents

11. Hájek M., Drahoš J.: Method of Drying Book and Similar Material. Pat. No. US 7,007,405. Applied: 03.12.30, Granted: 06.03.07.
12. Hájek M., Drahoš J., Volf V., Vozáb J.: Sposob y apparat dlya tēplovoi obrabotki stēklyannykh materialov i prirodnykh materialov vulkanicheskogo proiskhozhđeniya. (Russ) Method and Apparatus for Heat Treatment of Glass Material and Natural Materials Specifically of Volcanic Origin. Pat. No. RU 2 267 464. Applied: 00.06.12, Granted: 06.01.17.
13. Hájek M., Drahoš J., Volf V., Vozáb J.: Sposob i urzadzenie do obrovki cieplnej materialow szklanych i materialow naturalnych zwlaszcza pochodzenia wulkaniczego. (Pol) Method and Apparatus for Heat Treatment of Glass Material Specifically of Volcanic Origin. Pat. No. PL-P.352861. Applied: 01.12.16, Granted: 06.07.21.
14. Hájek M., Drahoš J., Volf V., Vozáb J.: Spōsob a zariadenie na tepelné spracovanie sklárskych materiālov a prirodnykh materiālov najme vulkanického pōvodu. (Slov) Method and Apparatus for Heat Treatment of Glass Material and Natural Materials Specifically of Volcanic Origin. Pat. No. SK 284512. Applied: 01.12.14, Granted: 06.06.12.
15. Hájek M., Círka V., Drahoš J., Ďurovič M., Paulusová H., Weberová L.: Zařizení pro vysoušení knižního a podobného papírového materiálu. (Czech) Equipment for Drying of Book and Similar Paper Material. Pat. No. PUV 2006-18008. Applied: 06.08.18, Granted: 06.10.02.

International conferences

16. Bunganič R., Růžička M., Drahoš J.: Dynamics of a Submerged Orifice. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 837, Praha, Czech Republic, 27-31 August 2006.
17. Cvetinović D., Tihon J., Vejrazka J., Drahoš J.: Turbulent Modelling of Circulat Jet Impinging of a Flat Plate and Its Validation by Hot-Wire Anemometry. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, pp. 849-850, Praha, Czech Republic, 27-31 August 2006.
18. Drahoš J., Růžička M.: Characterization of Process Data by Time Series Analysis. South African Chemical Engineering Congress 2006, Book of Abstracts, p. 46, Durban, South Africa, 20-22 September 2006.
19. Fialová M., Staykov P., Vlaev S.D.: Local Flow Field Characterization of a Bubble Column Generated by CFD. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 836 (9 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
20. Fujasová M., Havlica J., Růžička M., Drahoš J.: Hydrodynamic of Bubble-Particle Interactions in Liquid Phase. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 775 (6 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.

21. Fujasová M., Havlica J., Růžička M., Drahoš J.: Single Bubble and Single Particle Interactions in Liquid Phase. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 264 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
22. Fujasová M., Moucha T., Linek V.: The Influence of Impeller Geometry on Mass Transfer in Gas-Liquid Dispersion with Multiple-Impellers. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 239 (7 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
23. Fujasová M., Vejražka J., Růžička M.: Experimentální studie interakcí bubliny s pevnou stěnou. (Czech) Experimental Study of Bubble Interactions with Wall. Colloquium FLUID DYNAMICS 2006, Proceedings, pp. 33-34, Prague, Czech Republic, 25-27 October 2006.
24. Gogová Z., Fujasová M., Hanika J.: Experimental Study of Catalyzed Wet Oxidation of Ethanol in a Stirred Slurry Reactor. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 251 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
25. Havlica J., Bunganič R., Růžička M., Drahoš J.: CFD Simulations of Bubble Formation at an Orifice and Needle. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 253, Tatranské Matliare, Slovakia, 22-26 May 2006.
26. Havlica J., Bunganič R., Růžička M., Drahoš J.: Bubble Formation: CFD Simulations and Experiments. Euromech Colloquium 479: Numerical Simulation of Multiphase Flow with Deformable Interfaces, Book of Abstracts, pp. 1-4, Scheveningen, Netherlands, 14-16 August 2006.
27. Havlica J., Bunganič R., Šimčík M., Růžička M., Drahoš J.: The Ability of CFD to Deal with the Bubble Formation at an Orifice. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 772, Praha, Czech Republic, 27-31 August 2006.
28. Hladil J., Růžička M.: Instabilities and Patterns in Sedimenting Complex Polydisperse Mixtures: Relevance for Geological Sediments. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 851, Praha, Czech Republic, 27-31 August 2006.
29. Hladil J., Růžička M.: Pattern Formation in Geological Sediments: Field Observations versus Experiments in a Glass of Water. EUROMECH Colloquium 477, Book -of- Abstracts, pp. 1-2, University of Twente, Netherlands, 21-23 June 2006.
30. Kristiawan M., Besombes C., Sobolík V., Allaf K.: Instant Controlled Pressure Drop (DIC) as a Process of Extraction of Volatile Oils: The Impact of the Rate of Pressure Drop. 37th International Symposium on Essential Oils, Program & Book of Abstracts, p. 40, Grasse - Opio, France, 10-13 September 2006.
31. Kristiawan M., Sobolík V., Allaf K.: Application of Instantaneous Auto-Vaporization Process for Essential Oil Extraction: Case of Indonesian Ylang-Ylang Flowers. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 462 (13 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
32. Macháčová K., Wichterle K., Večeř M.: Motion Periodicity of Wobbling Ellipsoidal Bubbles. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 270 (5 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
33. Orvalho S., Fialová M., Fujasová M., Drahoš J., Růžička M.: Volumetric Mass Transfer Coefficient and Gas Holdup in Bubble Column. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 292 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
34. Orvalho S., Fialová M., Fujasová M., Drahoš J., Růžička M.: Application of Dynamic Pressure Step Method for $k_L a$ Measurement in Bubble Column. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 787 (7 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
35. Paglianti A., Fujasová M., Montante G.: Experimental Study and a Mechanistic Model on the Effect of Ventilated Cavities in Gassed Stirred Vessels. 12th European Conference on Mixing, Proceedings, pp. 145-152, Bologna, Italy, 27-30 June 2006.

36. Pěnkavová V., Tihon J.: The Effect of Channel Geometry on a Backward-Facing Step Flow. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 262, Tatranské Matliare, Slovakia, 22-26 May 2006.
37. Pěnkavová V., Tihon J.: The Effect of Inlet Flow Pulsations on the Flow Structure behind a Backward-Facing Step. Colloquium FLUID DYNAMICS 2006, Proceedings, pp. 91-94, Praha, Czech Republic, 25-27 October 2006.
38. Plzáková M., Večeř M., Růžička M., Drahoš J.: Effects of Electrolytes on Stability of Homogeneous Regime in Bubble Columns. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 263 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
39. Rochová K., Sovová H., Sobolík V., Allaf K.: Impact of Seed Structure Modification on the Rate of Supercritical CO₂ Extraction. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 2, p. 481 (8 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
40. Růžička M., Večeř M., Orvalho S., Drahoš J.: Dual Effect of Surface Active Agent on Stability of Uniform Flow Regime in Bubble Column. 4th Japanese-European Two-Phase Flow Group Meeting, Proceedings, p. 1 (8 pp. full text on CD-ROM), Kanbaikan, Kyoto, Japan, 24-28 September 2006.
41. Stanovský P., Vejražka J., Růžička M., Drahoš J.: Dynamics of a Vertically Aligned Bubbles. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 265 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
42. Stanovský P., Vejražka J., Růžička M., Drahoš J.: Hydrodynamic Interactions of Bubbles Rising in Vertical Arrangement. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 695, Praha, Czech Republic, 27-31 August 2006.
43. Stanovský P., Vejražka J., Růžička M., Drahoš J.: Hydrodynamic Interactions between in-Line Rising Bubbles. Colloquium FLUID DYNAMICS 2006, Proceedings, pp. 117-118, Prague, Czech Republic, 25-27 October 2006.
44. Stanovský P., Vejražka J., Růžička M., Drahoš J., Sanada T., Watanabe M.: A Case Study on Control Bubble Production and Bubble-Bubble Interactions. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 824, Praha, Czech Republic, 27-31 August 2006.
45. Staykov P., Fialová M., Vlaev S.D.: CFD Simulation of Bubble Column: Effect of Gas Distributor. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 283 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
46. Šimčík M., Večeř M., Havlica J., Růžička M., Drahoš J., Cartellier A., Wichterle K.: Gas Holdup Distribution in 2D Bubble Column: Experiments and CFD Simulations. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 261 (7 pp. full text on CD-ROM), p. 261, Tatranské Matliare, Slovakia, 22-26 May 2006.
47. Šimčík M., Večeř M., Havlica J., Růžička M., Drahoš J., Cartellier A.: Flow Properties in 2D Bubble Column Reactors: Experiments vs. CFD Simulations. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, P1.007, p. 781, Praha, Czech Republic, 27-31 August 2006.
48. Večeř M., Kulaviak L., Šimčík M., Růžička M., Drahoš J., Wichterle K.: Characterization of Local Properties of Bubble Bed by Optical Fiber Probes. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 260 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
49. Večeř M., Plzáková M., Růžička M., Drahoš J.: Influence of Surface Active Agents on Transition of Flow Regimes in Bubble Columns. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 784, Praha, Czech Republic, 27-31 August 2006.
50. Večeř M., Růžička M., Drahoš J.: Influence of Bubble Size on Stability of Homogeneous Flow Regime in Bubbly Columns. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 783, Praha, Czech Republic, 27-31 August 2006.

51. Večeř M., Šimčík M., Růžička M., Drahoš J., Cartellier A., Wichterle K.: Coherent Flow Structures in Flat Bubble Column Reactors. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 92 (2 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
52. Vejražka J., Fujasová M., Stanovský P.: Bubble Detachment Controlled by Needle Movement. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 697, Praha, Czech Republic, 27-31 August 2006.
53. Vejražka J., Fujasová M., Stanovský P.: Detachment of Bubbles from an Oscillating Needle. EFMC6 -EUROMECH Fluid Mechanics Conference 6, Abstracts, p. 411, Stockholm, Sweden, 26-30 June 2006.
54. Vejražka J., Stanovský P., Fujasová M.: Tvorba bublin řízená pohybem jehly. (Czech) Bubble Production Controlled by Needle Movement. Colloquium FLUID DYNAMICS 2006, Proceedings, pp. 141-144, Prague, Czech Republic, 25-27 October 2006.
55. Vejražka J., Stanovský P., Fujasová M., Růžička M., Drahoš J.: Control of Bubble Production from a Needle. 7th German/Japanese Symposium on Bubble Columns, Programme, p. 1 (6 pp. full text on CD-ROM), Goslar, Germany, 20-23 May 2006.
56. Wein O., Tihon J., Tovčigrečko V., Sobolík V.: Effect of Insulating Gaps on the Dynamic of Electrodiffusion Friction Probes. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 812, Praha, Czech Republic, 27-31 August 2006.
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59. Wichterle K., Macháčová K., Raška P., Večeř M.: Experimental Study of the Period Oscillation of Rising Bubbles. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, 696 (12 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
60. Wouahbi F., Havlica J., Allaf K., Sobolík V.: Mapping of Couette-Taylor Flow by Electrodiffusion Method. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 3, p. 734 (13 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.

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
- Butadiene-siloxane block copolymers
- Microwave activation of heterogeneous catalytic reactions
- Effect of microwave radiation on photochemical reactions
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphasic media
- Carbosilane dendrimers

Applied research

- Simultaneous disinfection and microwave drying of books and similar paper-based materials
- Microwave technology for production of new glasses
- Complex dehalogenation of PCB contaminated soils, waste water and oils

Research projects

Research and verification of methods of catalytic dehalogenation of contaminated groundwater on bimetallic permeable barriers

(F.Kaštánek, supported by Ministry of industry and trade, project No. FI-IM3/050)

The project deals with development and application of two methods for a decontamination of waste and underground water polluted by variety of hazardous halogenated organic substances. The decomposition of organic substances by active radicals

(Fenton reaction under the action of UV-irradiation) and by reductive dehalogenation (dehalogenation of organics on metallic Pd deposited on different supports at the presence of zero-valent iron-Pd/Fe) has been studied. [Refs. 11-14, 18, 37]

Microwave activation of heterogeneous catalytic reactions

(M. Hájek, supported by ICPF)

Research has been focused on the microwave activation of heterogeneous catalytic reactions in liquid phase where reactants are transparent to microwaves and the catalyst is the only compound, which couples with microwaves. It was found that selectivity of catalytic reactions can be efficiently improved when the surface of catalyst is superheated by microwaves and reaction mixture is simultaneously cooled. Application of microwave effects in heterogeneous catalysis has been examined. [Ref. 34]

Microwave technology for production of new glasses

(M. Hájek, supported by ICPF)

A new technology for melting and manufacture of glass has been applied to production of new kinds of glasses. [Refs. 21-25]

Effect of microwave radiation on photochemical reactions

(M. Hájek, supported by ICPF)

Reactions under simultaneous MW-UV irradiations have been studied using electrodeless UV lamps and compared to reactions under conventional UV radiation. New electrodeless lamps have been prepared generating different wavelengths. [Refs. 1, 42]

Microwave drying and disinfection of books

(M. Hájek, supported by ICPF)

New technology of simultaneous disinfection and microwave drying of books and paper-based materials has been optimised and applied for patent protection in EU, USA and Canada. Continuous microwave dryer with capacity of 100 dried books per day has been successfully tested. [Ref. 20, 26, 35]

Novel fluorophilic ligands for transition metal complexes

(J. Čermák, supported by Ministry of Education, grant No. LC06070)

Chemistry of $[(C_5Me_4C_nF_{2n+1})Rh]$ fragment was investigated in detail, allowing a semiquantitative assessment of steric properties of the tetramethyl(perfluoroalkyl)cyclopentadienyl ligands. The comparison of fluorophilicity of fluorous cyclopentadienes of various types and their rhodium and titanium complexes showed unusually high fluorophilicity of some complexes with very low fluorine content. [Ref. 7, 8, 29, 30, 44-46, 50]

New catalysts based on diphosphinoazine complexes

(J. Čermák, supported by Ministry of Education, grant No. LC06070)

Complexes of diphosphinoazines with various late transition metals were found to catalyze organic C-C coupling reactions as well as some H-X additions on double bonds like hydroamination and hydroformylation. Catalytic studies were supported by stoichiometric reactions documenting the principle modes of activation of organic molecules and by quantum chemical calculations in some cases. [Refs. 4-6, 40, 41]

Carbosilane dendrimers for catalytic applications

(J. Čermák, supported by Ministry of Education, grant No. LC06070)

Carbosilane dendrimers of zeroth to second generation were synthesized by different strategies and with various substitutions on the periphery. The dendrimers were characterized by multinuclear NMR and MALDI-TOF mass spectroscopy methods. [Ref. 15]

Novel organic-inorganic materials in opto-electronic systems for the monitoring and control of bio-processes

(G. Kuncová, supported by EC, grant No. GRD-2001-40477/ MATINOES)

Optical sensors of oxygen and glucose were tested in a bioreactor during cultivation. The influence of structure of ruthenium complexes on oxygen, glucose sensitivity and glucose concentration range was demonstrated. [Refs. 27, 28, 38, 39, 43]

Combined process for methyl tert-butyl ether (MTBE) removal from water

(G. Kuncová, joint project with ICT, supported by GA CR, grant No. 104/05/2637)

Fixed bed bioreactor with bacterial consortium degrading MTBE, named NEM, was build up. After one month free cells decreased content of MTBE about 20% while biodegradation with silica immobilized cells was not observed. During one year period changes in composition of bacterial consortium fed only with MTBE and methanol were monitored. The new route of preparation of polydimethylsiloxanes, perspective carriers for applications in biotechnologies was developed. [Ref. 9, 31-33, 47, 48]

Singlet oxygen producing sensitizers on solid inorganic hosts: photodisinfecting materials and probes

(G. Kuncová, joint project with Institute of Inorganic Chemistry and J. Heyrovsky Institute of Physical Chemistry of the ASCR, and CU, supported by GA CR, grant No. 203/06/1244)

The core of the project is design, preparation, characterization and final testing of novel photoactive materials. These materials consist of singlet oxygen 1O_2 producing photosensitizers intercalated into layered materials (smectites, hydrotalcites) or embedded into silica matrices. The same sensitizers will be embedded into silica sol-gel matrices. The results will be correlated with the characteristics of the host material and used for probing the matrices for enzymatic reactions. Generation of 1O_2 assigns the materials as well for application as photo-disinfecting and cell killing materials.

Interaction of organic-inorganic matrices with immobilized biological material

(G. Kuncová, COST Action 865: Bioencapsulation Multiscale Interaction Analysis. Project supported by the Ministry of Education, grant No. OC121)

The research has been focused on immobilization of enzyme lipase and cells degrading environmental pollutants. Cells degrading phenol, polychlorinated biphenyls, polyaromates and methyl tert-butyl ether have been immobilized and applied in bioreactors for biodegradation of pollutants in contaminated water and construction of whole cells biosensors of environmental pollutants. [Ref. 2, 19]

International co-operations

Instituto Superior 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

Centro de Engenharia Biológica, Universidade do Minho, Braga, Portugal: Monitoring of viability of immobilized cells by optical methods

Universidade Nova de Lisboa, Lisbon: Immobilization of lipase and cutinase on inorganic supports

Visitors

D.K. Agrawal, The Pennsylvania State University, USA

R.S. Varma, U.S. Environmental Protection Agency, Cincinnati, USA

Teaching

F. Kaštánek: ICT, course "Bioengineering"

J. Čermák: J. E. Purkyně University, Ústí n. L., courses "Organic Chemistry I" and "Organic Chemistry II"

Publications

Original papers

1. Církva V., Vlková L., Relich S., Hájek M.: Microwave Photochemistry IV: Preparation of the Electrodeless Discharge Lamps for Photochemical Applications. *J. Photochem. Photobiol., A* 179(1-2), 229-233 (2006).
2. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus : Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.* 38(2), 121-131 (2006).
3. Kaštánek F., Hanika J.: Úloha chemického inženýrství ve zvyšování bezpečnosti chemických výrob. (Czech) The Role of Chemical Engineering in Enhancement of Chemical Process Safety. *Chem. Listy* 100(2), 150-155 (2006).
4. Pošta M., Čermák J., Vojtíšek P., Císařová I.: Diphosphinoazine Rhodium(I) and Iridium(I) Complexes. *Collect. Czech. Chem. Commun.* 71(2), 197-206 (2006).
5. Včelák J., Čermák J., Czakoová M., Storch J.: Hydroamination of Methyl Methacrylate Catalyzed by Cationic Palladium Diphosphinoazine Complexes. *J. Mol. Catal. A-Chem.* 259(1-2), 41-45 (2006).
6. Carvalho M.F., Čermák J., Fernandes A.C., Ferreira A.S., Galvao A.M., Matos I., Marques M.M.: Ethylene Polymerisation by Ni-Diphosphine Azine Complexes. *Polym. Int.*, in press.
7. Čermák J., Žádný J., Krupková A., Lopatová K., Vlachová A., Nguyen Thi T.H., Šauliová J., Sýkora J., Císařová I.: Tetramethyl(perfluoroalkyl)cyclopentadienyl Rhodium(III) Complexes Containing Phosphorus and Nitrogen Monodentate Donors. Crystal Structure of $[(\eta^5\text{-C}_5\text{Me}_4\text{C}_4\text{F}_9)\text{Rh}(\text{PPri}_3)\text{Cl}_2]$. *J. Organomet. Chem.*, submitted.
8. Červenková Šťastná L., Auerová K., Kvíčala J., Čermák J.: Fluorophilic Properties of (Perfluorooctyl)Ethyltrimethylsilyl Substituted and Tetramethyl(Perfluoroalkyl) Substituted Cyclopentadienes and Their Ti(IV), Rh(III), and Rh(I) Complexes. *J. Organomet. Chem.*, submitted.

9. Gavlasová P., Kuncová G., Macková M.: Approaches to Design Whole Cell Biosensors for PCB Analysis Based on Optical Detection. Biodegradation, submitted.
10. Hájek M.: Microwave Drying of Paper Documents. Ceram. Trans., submitted.
11. Kaštánek F.: System of Decontamination of Wastes Containing PCBs. J. Hazard. Mater., in press.
12. Kaštánek F., Maléterová Y., Kaštánek P.: Zdroje rizik při aplikaci technologií na zneškodňování nebezpečných odpadů. (Czech) Safety Risks in Technologies for Decontamination of Hazardous Wastes. Chem. Listy, submitted.
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14. Kaštánek F., Páca J., Maléterová Y.: Biodegradation of Phenol at the Presence of Polyaromatic Hydrocarbons (PAH) in Soil. Int. Biodeterior. Biodegrad., submitted.
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16. Leitmannová E., Storch J., Červený L.: Selective Two-Phase Hydrogenations of Sorbic Acid Using Cp*Ru(sorbic acid)]⁺ Catalyst. React. Kinet. Catal. Lett., submitted.
17. Šabata S., Blechta V., Karban J., Pleska A., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. Phosphorus, Sulfur and Silicon, submitted.
18. Kaštánek F., Maléterová Y., Kaštánek P., Rott J., Jiříčný V., Jirátová K.: Complex Treatment of Wastewater and Groundwater Contaminated by Halogenated Organic Compounds. Desalination, in press.
19. Trögl J., Kuncová G., Kubicová L., Pařík P., Hálová J., Demnerová K., Ripp S., Saylor G.S.: Effect of Naphthalene and Salicylate Analogues on the Bioluminescence of Bioreporter *Pseudomonas Fluorescens* HK44. Folia Microbiol., in press.

Patents

20. Hájek M., Drahoš J.: Method of Drying Book and Similar Material. Pat. No. US 7,007,405. Applied: 03.12.30, Granted: 06.03.07.
21. Hájek M., Drahoš J., Volf V., Vozáb J.: Sposob i aparat dlya teplovoi obrabotki steklyannykh materialov i prirodnykh materialov vulkanicheskogo proischozhdeniya. (Russ) Method and Apparatus for Heat Treatment of Glass Material and Natural Materials Specifically of Volcanic Origin. Pat. No. RU 2 267 464. Applied: 00.06.12, Granted: 06.01.17.
22. Hájek M., Drahoš J., Volf V., Vozáb J.: Sposob i urzadzenie do obrovki cieplnej materialow szklanych i materialow naturalnych zwlaszcza pochodzenia wulkaniczego. (Pol) Method and Apparatus for Heat Treatment of Glass Material Specifically of Volcanic Origin. Pat. No. PL-P.352861. Applied: 01.12.16, Granted: 06.07.21.
23. Hájek M., Drahoš J., Volf V., Vozáb J.: Spôsob a zariadenie na tepelné spracovanie sklárskych materiálov a prírodných materiálov zvlášť vulkanického pôvodu. (Slov) Method and Apparatus for Heat Treatment of Glass Material and Natural Materials Specifically of Volcanic Origin. Pat. No. SK 284512. Applied: 01.12.14, Granted: 06.06.12.
24. Smrček J., Hájek M., Vilík P.: Method and Apparatus for Homogenization of Melt. Pat. No. EP 1 456 138. Applied: 02.11.15, Granted: 06.09.27.
25. Smrček J., Hájek M., Vilík P.: Method and Apparatus for Homogenization of Melt. Pat. No. ZL 0282688.7. Applied: 02.11.15, Granted: 06.07.26.
26. Hájek M., Církva V., Drahoš J., Ďurovič M., Paulusová H., Weberová L.: Zařízení pro vysoušení knižního a podobného papírového materiálu. (Czech) Equipment for Drying of Book and Similar Paper Material. Pat. No. PUV 2006-18008. Applied: 06.08.18, Granted 06.10.02.

International conferences

27. Bolyó J., Kuncová G.: Optical Monitoring of Oxygen Concentration and Cells Viability in Polymer Film with Entrapped Cells. 14th International Workshop on Bioencapsulation and

- COST 865 Meeting, Book of Abstracts, pp. 195-198, Lausanne, Switzerland, 05-07 October 2006.
28. Bolyó J., Kuncová G.: Temperature Dependence of Optical Oxygen Sensor in Biofilm. 10th International Symposium on the Genetic of Industrial Microorganisms, Book of Abstracts, p. P 314, Prague, Czech Republic, 24-28 June 2006.
 29. Čermák J., Auerová K., Bříza T., Šťastná L., Žádný J., Kvíčala J.: Fluorous Cyclopentadienes and Cyclopentadienyls. 8th International Symposium on Biotechnology, Metal Complexes and Catalysis, Abstracts, pp. 83-84, Haikou, China, 06-09 November 2006.
 30. Čermák J., Žádný J., Vojtíšek P.: Rhodium(III) Complexes with $[(C_5Me_4C_nF_{2n+1})Rh]$ Fragment for Potential Use in Fluorous Biphasic Media and Supercritical CO_2 . CAPE Organometallic Symposium Organometallics and Their Applications (OATA), Programme and Abstracts, p. 33, Cape Town, South Africa, 09-11 August 2006.
 31. Gavlasová P., Kuncová G., Macková M.: Whole-Cell Optical Biosensor for PCBs. Photon06: Optics and Photonics 2006, Abstract Book, pp.83-84 (6 pp. full text), Manchester, Great Britain, 04-07 September 2006.
 32. Gavlasová P., Kuncová G., Macková M.: Approaches to Design Whole Cell Biosensor for PCB Analysis Based on Optical Detection. Trends in Ecotoxicology. Emerging Pollutants: Endocrine Disrupting Substances, Pharmaceutical and Personal Care Products, Scientific Programme, pp. 27-28, Gliwice, Poland, 03-04 April 2006.
 33. Gavlasová P., Kuncová G., Macková M.: Optical Detection of PCBs by Pseudomonas species 2. 10th International Symposium on the Genetic of Industrial Microorganisms, Book of Abstracts, p. P 309, Prague, Czech Republic, 24-28 June 2006.
 34. Hájek M.: Microwave Effects in Heterogeneous Catalysis. 3rd International Conference on Microwave Chemistry, Book of Abstracts, p. OC-15, Brno, Czech Republic, 03-07 September 2006.
 35. Hájek M., Ďurovič M., Paulusová H., Weberová L.: Microwave Drying and Disinfection of Paper Documents. 15th International Drying Symposium, Proceedings, pp. 1042-1047, Budapest, Hungary, 20-23 August 2006.
 36. Hájek M., Ďurovič M., Paulusová H., Weberová L.: Microwave Drying and Disinfection of Paper Documents. 15th International Drying Symposium IDS 2006, Proceedings, p. 1042, Budapest, Hungary, 20-23 August 2006.
 37. Kaštanek F., Maléterová Y., Kaštanek P.: Combination of Advanced Oxidation and/or Reductive Dehalogenation and Biodegradation for the Decontamination of Waters Contaminated with Chlorinated Organic Compounds. Environmental Applications of Advanced Oxidation Processes, Book of Abstracts p. 296 (10 pp. full text on CD-ROM), Chania, Greece, 07-09 September 2006.
 38. Kuncová G., Betancour L., Rose K., Scully P., Sašek L., Bolyó J., Brányik T., Spáčil J., Podrazký O., Matějec V., Jaffrezic-Renault N., Dzyadevych S.V.: Application of Encapsulation into UV Curable ORMOCER in a Construction of Optical Sensors. XIV International Workshop on Biocapsulation and COST 865 Meeting, Book of Abstracts, pp. 85-88, Lausanne, Switzerland, 05-07 October 2006.
 39. Matějec V., Mrázek J., Dzyadevych S.V., Podrazký O., Rose K., Kuncová G., Šašek L.: Optical Fibre Biosensor for Oxygen and Glucose Monitoring Based on Ruthenium/ORMOCER®/Enzyme Layers. Photon 06: Optics and Photonics 2006, Abstract Book, 13-14 (6 pp. full text), Manchester, Great Britain, 04-07 September 2006.
 40. Pošta M., Čermák J., Vojtíšek P., Císařová I.: Diphosphinoazine Rhodium(I) and Iridium(I) Complexes. 1st European Chemistry Congress, Abstract Book, p. 368, Budapest, Hungary, 27-31 August 2006.
 41. Pošta M., Storch J., Sýkora J., Císařová I., Vojtíšek P., Čermák J.: Coordination Behaviour of Diphosphinoazine Ligands in Rhodium and Iridium Complexes. XXII International Conference on Organometallic Chemistry, Poster Presentations, P71, p. 259, Zaragoza, Spain, 23-28 July 2006.
 42. Relich S., Církva V., Vlková L., Hájek M.: Photochemistry in the Microwave Oven: Preparation, Evaluation and Applications of the Electrodeless Discharge Lamps. 3rd International Conference

- on Microwave Chemistry, Book of Abstracts, p. PO-21, Brno, Czech Republic, 03-07 September 2006.
43. Rose K., Fernandez-Lafuente R., Dzyadevych S., Jaffrezic N., Kuncová G., Matějec V., Scully P.: Hybrid Coatings as Transducers in Optical Biosensors for Oxygen and Glucose Monitoring. Photon 06: Optics and Photonics 2006, Abstract Book, 24 (7 pp. full text), Manchester, Great Britain, 04-07 September 2006.
 44. Šťastná L., Auerová K., Čermák J., Kvičala J.: Fluorophilic Properties of Some Polyfluorinated Cyclopentadienyls and Their Titanium and Rhodium Complexes. Green Solvents for Processes, Book of Abstracts, p. 83, Friedrichshafen, Germany, 08-11 October 2006.
 45. Šťastná L., Auerová K., Kvičala J., Čermák J.: Fluorophilic Properties of Fluorinated Cyclopentadienes and Their Complexes with Titanium and Rhodium. XXII International Conference on Organometallic Chemistry ICOMC 2006, Poster Presentations, p. 352, Zaragoza, Spain, 23-28 July 2006.
 46. Šťastná L., Čermák J., Kvičala J.: Fluorophilic Properties of Some Polyfluorinated Cyclopentadienyls and Their Titanium and Rhodium Complexes. 15th International Symposium on Homogeneous Catalysis, Book of Abstracts, p. B25, Sun City, South Africa, 20-25 August 2006.
 47. Trögl J., Hálová J., Kuncová G., Kubicová L., Pařík P., Demnerová K., Ripp S., Sayler S.: Kvantitativní vztah mezi strukturou analogů naftalenu a salicylové kyseliny a bioluminiscenci *Pseudomonas Fluorescens* HK 44. (Czech) Quantitative Relation between Structure of Naphthalenes and Salicylic Acids and Bioluminescence of *Pseudomonas Fluorescens* HK44. 26. Vedecká Konferencia Priemyselná Toxikológia 06, Zborník Príspevkov, str. 17-18, Piešťany, Slovakia, 23-25 May 2006.
 48. Trögl J., Kuncová G., Kubicová L., Pařík P., Hálová J., Demnerová K., Ripp S., Sayler G.S.: Free and Immobilized Bioreporter *Pseudomonas fluorescens* KH44. Selectivity of Bioluminescence Response. 9th World Congress on Biosensors BIOSENSORS 2006, Delegate Manual, p. P93, Toronto, Canada, 10-12 May 2006.
 49. Trögl J., Kuncová G., Kubicová L., Pařík P., Hálová J., Demnerová K., Ripp S., Sayler G.S.: QASAR of Naphthalene and Salicylate Analogues for Monitoring Environmental Pollution. Slovak and Czech Toxicology in the European Union, Programme and Abstracts, p. 64, Trenčianské Teplice, Slovakia, 05-07 June 2006.
 50. Žádný J., Krupková A., Vlachová A., Císařová I., Sýkora J., Čermák J.: Synthesis of $[(C_5Me_4C_nF_{2n+1})RhLX_2]$ Complexes with Series of Phosphines and Nitrogen Ligands and NMR Study of Their Conformational Dynamics. XXII International Conference on Organometallic Chemistry, Poster Presentations, p. 421, Zaragoza, Spain, 23-28 July 2006.

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

Applied research

- Dechlorination of persistent organic pollutants
- Recovery of precious metals
- PET recycling
- Electronic scrap recycling

Research projects

Optimization of off-gas cleaning system with safe and reliable dioxin destruction

(V. Pekárek, supported by EUREKA OE 200)

Application of a new revolutionary technology developed by W.L. GORE & Associates, Ltd. to safely destroy dioxins and furans contained in off-gas from a municipal solid waste (MSW) incinerator based on catalytic filtration. Experiments were performed for destruction of POP compounds on fly ash from bag filters by CMD method originally developed in our laboratory. The CMD method was also successfully used for decontamination of extremely toxic samples containing PCBs and polychlorinated terphenyls in asphaltic residues. [Refs. 9, 10, 18, 19, 35-38, 43-45]

Gasification of biomass in fluidized bed – a source of renewable energy

(M. Punčochář, supported by GA CR 104/04/0829)

The project is motivated by effort to contribute to the development of alternative sources of small and medium power engineering. The project deals, in a complex way, with the problems arising in the gasification of typical biofuels in fluidized bed reactors. The blended fuel comprising coal and PET, which was chosen as a model component of waste plastics, in the bulk of brown coal was gasified in the atmospheric fluidized bed gasifier of laboratory-scale. The influence of bed and freeboard temperature on produced gas composition was compared with single coal gasification. [Refs. 11, 17, 20, 21, 23, 30, 32-34, 40-42, 46]

Demonstration of the production and utilization of synthetic natural gas from solid biofuels

(M. Punčochář, supported by STREP, TREN/05/FP6EN/S07.56632/019895)

Methane derived from solid biofuels is an important option for achieving the goal for an increased use of alternative motor fuels. The biomass methanation has already been demonstrated on the small scale. Methane can easily be fed into the existing Natural Gas infrastructure, and can then be used with available technology, in particular within vehicle fleets. Thus, the objective of the presented project is to realise and demonstrate the production of Synthetic Natural Gas (SNG) from solid biofuels within an innovative, large scale gasification plant which is in operation in Austria and to applicate this motor fuel in energy efficient vehicles (WTW).

Combustion of sewage sludge in the circulating fluidized bed

(M. Hartman, supported by GA ASCR, grant No. A4072201)

The proposed research is orientated towards resolving the burdensome difficulties with current disposal of voluminous digested sewage sludge. The project addresses most relevant issues related to its combustion such as very high contents of moisture, volatile matter and nitrogen, the presence of heavy metals, emissions of pollutant gases as well as the handling of solid by-products. [Refs. 4 -8, 12 – 16, 22, 24, 29, 31]

Preparation of the electrodeless discharge lamps for photochemical applications

(V. Církva, supported by GA CR 104/06/0992)

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, 3, 25, 26, 28, 39]

International co-operations

Vienna University of Technology, Vienna, Austria: 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

Visits abroad

K. Svoboda: Institute for Energy, Joint Research Centre of European Commission, Petten, The Netherlands (12 months)

Publications

Original papers

1. Brechler J., Pekárek V., Tydlitát V., Janota J.: Případová studie rozptylu par rtuti z bodového zdroje. (Czech) A Case Study of Mercury from Point Source. *Ochrana ovzduší* 19(1), 13-14 (2006).
2. Církva V., Duchek J., Kaplánek R., Paleta O., Michálek J., Přádný M., Chmelíková D., Wichterlová J.: New Perfluoroalkylated Amphiphilic Methacrylates Bearing Sulfinyl Group as Monomers for Biomedical Applications: Water Content and Oxygen Permeability of Their Copolymers with DEGMA. *Eur. J. Med. Chem.* 41(11), 1320-1326 (2006).
3. Církva V., Vlková L., Relich S., Hájek M.: Microwave Photochemistry IV: Preparation of the Electrodeless Discharge Lamps for Photochemical Applications. *J. Photochem. Photobiol., A* 179(1-2), 229-233 (2006).
4. Hartman M.: Letter to the Editor. Three-dimensional Modeling of a Circulating Fluidized-Bed Gasifier for Sewage Sludge. *Chem. Eng. Sci.* 61(12), 4132-4133 (2006).
5. Hartman M., Pohořelý M., Trnka O.: Chemická a palivová charakteristika anaerobně stabilizovaného čistírenského kalu a jeho popela. (Czech) Chemical and Fuel Characteristics of the Anaerobically Stabilized Sewage Sludge and Its Ash. *Chem. Listy* 100(9), 813-820 (2006).
6. Hartman M., Pohořelý M., Trnka O.: Transport Velocities of Different Particulate Materials in Pneumatic Conveying. *Chem. Pap.* 60(1), 74-77 (2006).
7. Hartman M., Trnka O.: Comments on "Ceria-Zirconia High-Temperature Desulfurization Sorbents". *Ind. Eng. Chem. Res.* 45(4), 1548-1549 (2006).
8. Hartman M., Trnka O., Svoboda K.: Impediment to Incipient Fluidization in Wet Beds of Porous Nonspherical Particles. *Chem. Eng. Commun.* 193(1), 100-115 (2006).
9. Pekárek V.: Spalování komunálních odpadů a jaderná energetika - ekologické problémy. (Czech) Municipal Waste Combustion and Nuclear Energetics - Ecologic Problems?. *Chem. Listy* 100(10), 861 (2006).
10. Pekárek V., Punčochář M., Šyc M., Pařízek T., Stehlík P., Bébar L., Oral J.: Aplikace katalytického filtru ve spalovně komunálního odpadu TERMIZO a.s. v Liberci pro snížení emisí perzistentních organických látek. (Czech) Application of Catalytic Filter in the Municipal Waste Incinerator Plant TERMIZO in Liberec for Lowering of Persistent Organic Compounds in Emissions. *Ochrana ovzduší* 19(4), 16-22 (2006).
11. Pohořelý M., Vosecký M., Hejdrová P., Punčochář M., Skoblia S., Staf M., Vošta J., Koutský B., Svoboda K.: Gasification of Coal and PET in Fluidized Bed Reactor. *Fuel* 85(17-18), 2458-2468 (2006).
12. Hartman M., Pohořelý M., Trnka O.: Fluidization of Dried Wastewater Sludge. *Powder Technol.*, submitted.
13. Hartman M., Pohořelý M., Trnka O.: The Behaviour of Inorganic Constituents of Municipal Sewage Sludge during Fluidized-Bed Combustion. *Chem. Pap.*, submitted.
14. Hartman M., Trnka O., Pohořelý M.: Minimum and Terminal Velocities in Fluidization of Particulate Ceramsite at Ambient and Elevated Temperature. *Ind. Eng. Chem. Res.*, submitted.
15. Hartman M., Trnka O., Pohořelý M.: Basic Fluidization Behavior of Oil-Contaminated Sand. *Chem. Pap.*, in press.

16. Hartman M., Trnka O., Pohořelý M.: Oxidace organického dusíku ve stechiometrických a bilančních výpočtech spalování stabilizovaného čistírenského kalu. (Czech) Oxidation of the Organic Nitrogen in Fuel-Lean Combustion Calculations of Sewage Sludge. Chem. Listy, in press.
17. Miccio F., Svoboda K., Schosger J.-P., Baxter D.: Biomass Gasification in Internal Circulating Fluidized Beds: a Thermodynamic Predictive Tool. Korean J. Chem. Eng., submitted.
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20. Svoboda K., Siewiorek A., Baxter D., Rogut J., Punčochář M.: Thermodynamic Possibilities and Constraints of Pure Hydrogen Production by a Chromium, Nickel and Manganese-Based Chemical Looping Process at Lower Temperatures. Chem. Pap., in press.
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22. Trnka O., Hartman M.: Vliv změn fyzikálních parametrů fluidních vrstev na charakteristiky tlakových fluktuací. (Czech) Influence of Changes in the Physical Parameters of Fluidized Beds on Its Characteristics of Pressure Fluctuations. Chem. Listy, submitted.

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23. Svoboda K., Baxter D., Martinec J.: Nitrous Oxide Emissions from Waste Incineration. Chem. Pap. 60(1), 78-90 (2006).
24. Hartman M., Trnka O.: Těžké kovy v čistírenském kalu a jejich chování při spalování. (Czech) Heavy Metals in Sewage Sludge and Their Behaviour in Incineration. Chem. Listy, in press.

Chapters in books

25. Klán P., Církva V.: Microwaves in Photochemistry. In: Microwaves in Organic Synthesis. (Loupy, A., Ed.), pp. 860-897, WILEY-VCH Verlag, Weinheim 2006.

Patents

26. Hájek M., Církva V., Drahoš J., Ďurovič M., Paulusová H., Weberová L.: Zařízení pro vysoušení knižního a podobného papírového materiálu. (Czech) Equipment for Drying of Book and Similar Paper Material. Pat. No. PUV 2006-18008. Applied: 06.08.18, Granted: 06.10.02.
27. Veselý V.: Způsob izolace kyseliny tereftalové. (Czech) Isolation Method of Terephthalic Acid. Pat. No. PV 2006-313. Applied: 06.05.16.

International conferences

28. Církva V.: Photochemistry in the Microwave Oven. 3rd International Conference on Microwave Chemistry, Book of Abstracts, p. OC-4, Brno, Czech Republic, 03-07 September 2006.
29. Hartman M., Trnka O., Pohořelý M.: Defluidization Tendency of a Wet Gas-Solid Fluidized Bed. 33rd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 243 (33 pp. full text on CD-ROM), Tatranské Matliare, Slovakia, 22-26 May 2006.
30. Hejdová P., Pohořelý M., Vosecký M., Skoblia S., Svoboda K., Vošta J., Punčochář M., Koutský B.: Effect of Experimental Conditions on Co-gasification of Coal and Polyethyleneterephthalate in Atmospheric Fluidized Bed Reactor. 19th International Conference on Fluidized Bed Combustion, Proceedings, pp. 1-9, Vienna, Austria, 21-24 May 2006.

31. Kameníková P., Pohořelý M., Vosecký M., Svoboda K., Skoblia S., Hartman M.: Emise oxidů dusíku při fluidním spalování mokřích stabilizovaných kalů. (Czech) NO_x Emissions from Fluidized Bed Combustion of Wet Sewage Sludge. 1. mezinárodní konference Zentiva z cyklu "Odpovědné podnikání v chemii", Praha, Czech Republic, 31 October 2006.
32. Kameníková P., Skoblia S., Vosecký M., Pohořelý M.: Comparison of Methods for Tar Sampling and Analysis. Methods for Alternative Fuel Production from Biomass and Waste, Sofie, Bulgaria, 19-20 October 2006.
33. Martinec J., Skála Z., Schosger J.-P., Baxter D., Svoboda K.: Development and Practical Tests of Insulating/Cooling Capsule with Sensor for In-situ Measurements of CO Concentrations on Moving Grates in MSWI. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 5, pp. 1698-1699 (18 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
34. Miccio F., Svoboda K., Schosger J.P., Baxter D.: Staged Gasification of Biomass and Wastes in Fluidized Bed. 19th International Conference on Fluidized Bed Combustion, Proceedings, p. 1-10, Vienna, Austria, 21-24 May 2006.
35. Ocelka T., Horák J., Tydlitát V., Pekárek V., Danihelka P., Grabic R., Obal L.: Emission of PCDD/Fs from Commercially Available Small Scale Appliances at Combustion of Various Oils. 26th International Symposium on Halogenated Persistent Organic Pollutants – DIOXIN2006, Organohalogen Compounds, Vol. 68, pp.2287-2290, Oslo, Norway, 21-25 August 2006.
36. Pekárek V., Bureš M.: Umožňuje termodynamický výpočet přispět k objasnění reakčního mechanismu?. (Czech) Is it Possible by Thermodynamic Equilibrium Calculations to Judge the Presumable Reaction Mechanism? 28. Mezinárodní slovenský a český kalorimetrický seminář 2006, Sborník příspěvků, pp. 29-32, hotel Poľana u Hriňové, Slovakia, 22-26 May 2006.
37. Pekárek V., Bureš M., Ocelka T.: The Copper Mediated Destruction of PCBs from the Standpoint of Thermodynamics Calculations. 4th PCB Workshop Recent Advances in the Environmental Toxicology and Health Effects of PCBs, Book of Abstracts, p. 30, Zakopane, Poland, 06-10 September 2006.
38. Pekárek V., Punčochář M., Bureš M., Grabic R., Fišerová E.: Equilibrium Calculations for Better Understanding of the Effects of SO₂ and H₂O₂ on the De novo Synthesis of PCDD/F in the N₂ + 10% O₂ Atmosphere Under Model Laboratory Conditions. 26th International Symposium on Halogenated Persistent Organic Pollutants – DIOXIN2006, Organohalogen Compounds, Vol. 68, pp.1224-1227, Oslo, Norway, 21-25 August 2006.
39. Relich S., Círka V., Vlková L., Hájek M.: Photochemistry in the Microwave Oven: Preparation, Evaluation and Applications of the Electrodeless Discharge Lamps. 3rd International Conference on Microwave Chemistry, Book of Abstracts, p. PO-21, Brno, Czech Republic, 03-07 September 2006.
40. Siewiorek A., Svoboda K., Rogut J.: Thermodynamic Possibilities of Pure Hydrogen Production by Chromium, Nickel and Manganese-Based Chemical Looping at Lower Temperatures. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 4, pp. 1340-1341 (17 pp. full text on CD-ROM), Czech Republic, 27-31 August 2006.
41. Svoboda K., Pohořelý M., Schosger J.-P., Baxter D., Rogut J.: Efficiency of Desulfurization in Sub-Stoichiometric Pressurized Fluidized Bed Combustion of Coals - Theoretical and Practical Problems. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 5, pp. 1719-1720 (20 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
42. Svoboda K., Slowinski G., Rogut J., Siewiorek A.: Thermodynamic Possibilities and Constraints for Pure Hydrogen Production by Iron Based Chemical Looping Process at Lower Temperatures. 17th International Congress of Chemical and Process Engineering CHISA 2006, Summaries 4, pp. 1338-1339 (20 pp. full text on CD-ROM), Praha, Czech Republic, 27-31 August 2006.
43. Šyc M., Pekárek V., Fišerová E., Punčochář M., Karban J., Prokeš O.: Catalytic Filter Application in the TERMIZO Municipal Solid Waste Incineration Plant in Liberec. 1. mezinárodní konference Zentiva z cyklu "Odpovědné podnikání v chemii", Praha, Czech Republic, 31 October 2006.

44. Šyc M., Pekárek V., Fišerová E., Punčochář M., Prokeš O.: Dioxinový filtr na spalovně komunálních odpadů TERMIZO a.s. (Czech) Catalytic Filter on Municipal Waste Incineration Plant TERMIZO a.s. Chemie energetických oběhů 6, Praha, Czech Republic, 11-12 September 2006.
45. Šyc M., Pekárek V., Fišerová E., Punčochář M., Karban J., Prokeš O.: Catalytic Filter Application in the TERMIZO Municipal Waste Incineration Plant in Liberec. 26th International Symposium on Halogenated Persistent Organic Pollutants – DIOXIN2006 , Organohalogen Compounds, Vol. 68, pp.1232-1235, Oslo, Norway, 21-25 August 2006.
46. Vosecký M., Pohořelý M., Kameníková P., Skobliá S., Koutský B., Punčochář M.: Biomass and Plastic Waste Gasification in Experimental Fluidized-Bed Gasifier. Methods for Alternative Fuel Production from Biomass and Waste, Book of Abstracts, Sofie, Bulgaria, 19-20 October 2006.

Laboratory of Aerosol Chemistry and Physics

Head: J. Smolík
Deputy: V. Ždímal
Research staff: D. Brus, P. Dohányosová, L. Džumbová, J. Kugler, V.V. Levdansky,
P. Moravec, J. Schwarz, I. Ševčíková, T. Trávníčková
PhD students: A. Hruška, D. Matějková, L. Štefancová

Fields of research

- Composition and size 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

Research projects

European Supersites for Atmospheric Aerosol Research

(J. Smolík, supported by EC, grant No. EVK4-CT-2002-00090 EUSAAR)

European infrastructure project of 6th FP. The project 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.

Indoor aerosol deposition: An experimental study

(J. Smolík, supported by GA CR, grant No. 101/04/1190)

The aim of the project is to study experimentally the deposition of aerosol particles in rectangular cavity at well-defined conditions. The measurements are conducted both with monodispersed and polydispersed aerosols at both low and high aerosol concentrations. Experiments are performed both for still air and turbulent conditions where the influence of ventilation rate, wall roughness, and ambient aerosol infiltrations is investigated. Laboratory tests were compared to the results obtained from measurements in real indoor environment (indoor living space). [Refs. 4, 18, 21, 23-26, 46-47]

Contribution of secondary atmospheric PM to total PM pollution loading

(J. Smolík, supported by Ministry of Environment, grant No. VaV-SM/9/86/05)

The project is aimed at characterisation of size-resolved atmospheric particulate matter (PM) in order to estimate the contribution of secondary atmospheric PM to the total PM pollution loading at suburban area of Prague. For this purpose one year semicontinuous PM sampling is performed with subsequent gravimetric and chemical analyses. The contribution of the inorganic part will be determined using ion chromatography. [Refs. 42, 48]

Composition of size-resolved atmospheric aerosol at Prague suburban area

(J. Smolík, supported by Ministry of Education, grant No. OC106)

The main task of the project is the development of humidity controlled inlets for cascade impactor and SMPS and APS systems. The inlets are used in study of hygroscopicity of size-resolved atmospheric particulate matter, sampled at suburban area of Prague. [Ref. 48]

Particulate matter: Properties related to health effects

(J. Smolík, supported by ESF, COST Action 633)

The project focuses on the development and evaluation of scientific methodologies and databases that would improve the scientific understanding and regulatory basis on the physico-chemical constituents and emission sources of ambient air particulate matter causing the current substantial mortality and morbidity among European populations. [Refs. 43, 44]

Development of experimental methods for measurement of nucleation rates in mixtures present in clean and polluted atmospheres

(V. Ždímal, supported by GA ASCR, grant No. IAA2076203)

Mainly experimental project focusing on development of methods studying nucleation kinetics in supersaturated vapours. It comprises four tasks: (i) Development of a laminar co-flow tube, a device to study binary nucleation using an entirely new method. Flow visualization was used to find the limits of stability and CFD methods were applied to compute the flow field. (ii) Improvement of the shock-tube method. (iii) Improvement of the static-diffusion-chamber method. (iv) Testing the experimental setups with selected systems. [Refs. 1, 5, 9, 20, 27-30, 38]

Metastable water and steam

(V. Ždímal, supported by GA CR, grant No. 101/05/2214)

The project aims to study the properties of water and steam in metastable state. In order to obtain missing engineering data and answer fundamental problems sophisticated experiments are carried out. A device is being developed for measurement of the surface tension of supercooled water. Studies on homogeneous nucleation from supercooled water vapor are going to be performed in an extended temperature range using a shock tube and a diffusion cloud chamber. Factors influencing the supercooling limit and the kinetics of freezing are studied. Water clusters, bulk supercooled liquid and its surface are simulated using Monte Carlo and molecular dynamics. Based on both experimental and simulation results, semi-phenomenological analytical models of metastable water and water clusters are developed, enabling engineering application. [Refs. 8, 31-37]

Application of new methods of aerosol measurement for investigation of the structure of the condensation nuclei in steam turbine

(V. Ždímal, supported by GA CR, grant No. 101/05/2524)

The goal of this project is to determine the real structure of the heterogeneous condensation nuclei in superheated (dry) steam. The structure of heterogeneous condensation nuclei co-determines the course of steam condensation in the turbine and thus influences its

energetic efficiency and the life-time of the blades. In this project, a unique approach is used to determine the structure of heterogeneous condensation nuclei, based on modern experimental methods and measuring devices, developed for investigation of atmospheric aerosol particles. A special sampling line is being developed to connect these devices, operating at laboratory conditions, to sampling ports of the turbine at high pressure and temperature. Experiments are carried out in laboratories and subsequently in a power plant. The results are compared with measured structure of the developed liquid phase, which depends on heterogeneous condensation nuclei, and with theoretical analysis. [Refs. 35, 36, 39]

Hygroscopic properties of urban and suburban carbonaceous aerosols

(J. Schwarz, Czech -Belgium bilateral exchange program in the frame of Czech -Flemish bilateral scientific cooperation.)

The aim of this project is to improve knowledge concerning-hygroscopic properties of atmospheric aerosols in an urban environment by joining capacities of both laboratories. Cascade impactors with constant humidity sampling inlets (dry and wet) are going to be used to obtain size resolved samples. These samples will be analysed using ion chromatography in Prague and then for water soluble carbon in Ghent laboratory. This attitude aims to assess the influence of water soluble organic carbon on hygroscopicity of separated size fractions of urban aerosols. [Ref. 48]

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

Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece: Urban aerosols. Modelling of transport processes in laminar diffusion cloud chamber: Comparison of methods determining atmospheric aerosol size distributions

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 characterisation 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

Visits abroad

L. Džumbová: Technical University of Crete, Chania, Greece (12 months)

Visitors

J. Marijnissen, TU Delft, Delft, The Netherlands

H. Keskinen, Institute of Physics, Tampere University of Technology, Tampere, Finland

W. Maenhaut, Ghent University, Institute for Nuclear Sciences, Ghent, Belgium

T. Hussein, Institute of Applied Environmental Science, Stockholm University, Stockholm, Sweden

Teaching

V. Ždímal: ICT, postgraduate course: "Aerosol Engineering"

Publications

Original papers

1. Brus D., Ždímal V., Stratmann F.: Homogeneous Nucleation Rate Measurements of 1-Propanol in Helium: The Effect of Carrier Gas Pressure. *J. Chem. Phys.* 124(16), Art. No. 6 (2006).
2. Bryant C., Eleftheriadis K., Smolík J., Ždímal V., Mihalopoulos N., Colbeck I.: Optical Properties of Aerosols Over the Eastern Mediterranean. *Atmos. Environ.* 40(32), 6229-6244 (2006).
3. Eleftheriadis K., Colbeck I., Housiadas C., Lazaridis M., Mihalopoulos N., Mitsakou C., Smolík J., Ždímal V.: Size Distribution, Composition and Origin of the Submicron Aerosol in the Marine Boundary Layer During the Eastern Mediterranean "SUB-AERO" Experiment. *Atmos. Environ.* 40(32), 6245-6260 (2006).
4. Hussein T., Glytsos T., Ondráček J., Dohányosová P., Ždímal V., Hameri K., Lazaridis M., Smolík J., Kulmala M.: Particle Size Characterization and Emission Rates During Indoor Activities in a House. *Atmos. Environ.* 40(23), 4285-4307 (2006).
5. Hyvärinen A.-P., Brus D., Ždímal V., Smolík J., Kulmala M., Viisanen V., Lihavainen H.: The Carrier Gas Pressure Effect in a Laminar Flow Diffusion Chamber, Homogeneous Nucleation of n-Butanol in Helium. *J. Chem. Phys.* 124(22), Art. No. 4 (2006).
6. Lazaridis M., Aleksandropoulou V., Smolík J., Hansen J.E., Glytsos T., Kalogerakis N., Dahlin E.: Physico-Chemical Characterization of Indoor/Outdoor Particulate Matter in Two Residential Houses in Oslo, Norway: Measurements Overview and Physical Properties – URBAN-AEROSOL Project. *Indoor Air* 16(4), 282-295 (2006).
7. Lazaridis M., Eleftheriadis K., Smolík J., Colbeck I., Kallos G., Drossinos Y., Ždímal V., Večeřa Z., Mihalopoulos N., Mikuška P., Bryant C., Housiadas C.: Dynamics of Fine Particles and Photo-Oxidants in the Eastern Mediterranean (SUB-AERO). *Atmos. Environ.* 40(32), 6214-6228 (2006).
8. Levdansky V.V., Smolík J., Moravec P.: Vliyanie razmernykh effektov na kriticheskii diametr i rost nanochastits. (Russ) Influence of Size Effects on Critical Diameter and Growth of Nanoparticles. *Inzh. - Fiz. Zh. [J. Eng. Phys. Thermophys.* 79(2), 217-221, 2006] 79(2), 14-18 (2006).
9. Levdansky V.V., Smolík J., Moravec P.: Influence of Size Effect and Foreign Gases on Formation of Nanoparticles. *Int. Commun. Heat Mass Transfer* 33(1), 56-60 (2006).

10. Levdansky V.V., Smolík J., Moravec P.: Free-Molecular Gas Flow in Channels (Pores) with Physico-Chemical Transformation on the Surface. *Int. J. Heat Mass Transfer* 49(13-14), 2356-2365 (2006).
11. Spyridaki A., Lazaridis M., Eleftheriadis K., Smolík J., Mihalopoulos N., Aleksandropoulou V.: Modelling and Evaluation of Size-Resolved Aerosol Characteristics in the Eastern Mediterranean during the SUB-AERO Project. *Atmos. Environ.* 40(32), 6261-6275 (2006).
12. Levdansky V.V., Dragun V.L., Smolík J., Ždímal V., Moravec P.: Vliyanie poverkhnostnykh effektov pri kondenzatsii para na nanorazmernoii chastitse imeyushchei elektricheskii zaryad. (Russ) Influence of Surface Effects on Vapor Condensation on Nanoscale Particle with Electric Charge. *Inzh. - Fiz. Zh. (J. Eng. Phys. Thermophys.)*, submitted.
13. Levdansky V.V., Smolík J., Moravec P.: Indutsirovannyi izlucheniem dreif vodoroda i ego zakhvat v metallicheskih membranakh i chastitsakh. (Russ) Radiation-Induced Drift of Hydrogen in Metallic Membranes and Particles. *Inzh. - Fiz. Zh.*, submitted.
14. Levdansky V.V., Smolík J., Moravec P.: Vliyanie postoronnikh gazov na fazovye perekhody v nanorozmernykh kapillyarakh. (Russ) Influence of Foreign Gases on Phase Transitions in Nanoscale Capillaries. *Inzh. - Fiz. Zh.*, submitted.
15. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Osobennosti fazovykh perekhodov pri formirovanii nanorozmernykh aerazolnykh chastits. (Russ) Features of Phase Transitions in Formation of Nanosize Aerosol Particles. *Inzh. - Fiz. Zh.*, submitted.
16. Moravec P., Smolík J., Keskinen H., Mäkelä J., Levdansky V.V.: Vapor Phase Synthesis of Zirconia Fine Particles from Zirconium tert-Butoxide. *J. Mater. Sci.*, submitted.
17. Moravec P., Smolík J., Keskinen H., Mäkelä J.M., Levdansky V.V.: ZrO₂/SiO₂ Fine Particle Synthesis by MOCVD. *Chem. Vapor Depos.*, submitted.
18. Smolík J., Dohányosová P., Schwarz J., Ždímal V., Lazaridis M.: Characterization of Indoor/Outdoor Aerosols in a Suburban Area of Prague. *Water, Air, Soil Pollut.*, submitted.
19. Večeřa Z., Mikuška P., Smolík J., Eleftheriadis K., Bryant Ch., Colbeck I., Lazaridis M.: Shipboard Measurements of Nitrogen Dioxide, Nitrous Acid, Nitric Acid and Ozone in the Eastern Mediterranean Sea. *Water, Air, Soil Pollut.*, submitted.

International conferences

20. Brus D., Ždímal V., Stratmann F.: Homogeneous Nucleation Rate Measurements of 1-Propanol in Helium, the Effect of Carrier Gas Pressure. 80th ACS Colloid and Surface Science Symposium, Abstracts, p. 242, Boulder, Colorado, USA, 18-21 June 2006.
21. Dohányosová P., Štefancová L., Ševčíková I., Kugler J., Moravec P., Schwarz J., Ždímal V., Smolík J., Hruška A.: Christmas Party Emissions. *NOSA 2006 Aerosol Symposium, Book of Abstracts*, pp. 66-68, Helsinki, Finland, 08-10 November 2006.
22. Eleftheriadis K., Vratolis S., Housiadas C., Smolík J., Ždímal V., Schwarz J., Wagner Z., Lazaridis M., Ondráček J., Hussein T., Kephelopoulos S., Drossinos Y.: Modal Structure of the Fine Urban Aerosol in Four European Cities. 7th International Aerosol Conference, Proceedings, p. 1786, St. Paul, Minnesota, USA, 10-15 September 2006.
23. Hruška A., Dohányosová P., Hemerka J., Smolík J.: Experimental Studies of the Aerosol Dynamic in the Test Chamber. *NOSA 2006 Aerosol Symposium, Book of Abstracts*, pp. 98-102, Helsinki, Finland, 08-10 November 2006.
24. Hruška A., Dohányosová P., Hemerka J., Smolík J.: Indoor Aerosol Deposition. 17th Air-Conditioning and Ventilation Conference 2006, Proceedings, pp. 103-107, Praha, Czech Republic, 17-19 May 2006.
25. Hruška A., Dohányosová P., Hemerka J., Smolík J.: Experimental Studies of the Aerosol Deposition in a Test Chamber. 5th International Conference of Advanced Engineering Design AED 2006, 8 pp. full text on CD-ROM, Praha, Czech Republic, 11-14 June 2006.
26. Hruška A., Dohányosová P., Hemerka J., Smolík J.: Experimental Studies of the Aerosol Deposition and Coagulation in a Test Chamber. *Advanced Atmospheric Aerosol Symposium, Chemical Engineering Transaction, Vol. 10*, pp. 465-470, Milano, Italy, 12-15 November 2006.

27. Hyvärinen A.-P., Brus D., Ždímal V., Lihavainen H.: Homogeneous Nucleation Kinetics Measurements in Supersaturated Vapors of n-Butanol, the Influence of Total Pressure. 7th International Aerosol Conference, Proceedings, p. 1624-1625, St.Paul, Minnesota, USA, 10-15 September 2006.
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43. Schwarz J., Smolík J., Hovorka J.: Ionic Composition of Atmospheric Aerosol PM10 Size Fraction at Prague Suburb. Advanced Atmospheric Aerosol Symposium, Chemical Engineering Transactions, Vol. 10, pp. 419-424, Milan, Italy, 12-15 November 2006.
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46. Smolík J., Schwarz J., Dohányosová P.: Composition of Indoor Particulate Matter. Healthy Buildings 2006, Proceedings, pp. 483-486, Lisboa, Portugal, 04-08 June 2006.
47. Smolík J., Ždímal V., Schwarz J., Lazaridis M., Dohányosová P.: Characterisation of Indoor/Outdoor Aerosols In Suburban Area Of Prague. Protection and Restoration of the Environment VIII, Book of Abstracts, p. 529-530, Chania, Greece, 03-07 July 2006.
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Laboratory of Laser Chemistry

Head: J. Pola
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Research staff: V. Dřínek, A. Galíková, J. Kupčík, D. Pokorná, M. Urbanová, P. Stopka
Technical staff: D. Bartlová
PhD student: J. Blazevska-Gilev, T. Křenek

Fields of research

- IR and UV laser induced chemistry
- IR and UV laser induced chemical vapour deposition of novel polymeric and Si-based materials
- UV laser-induced polymerization in the gas phase
- UV laser-induced photolysis of organosilicon, organoselenium and organotellurium compounds
- IR and UV laser induced ablation of polymers
- UV laser chemical deposition of nanosols and nanocomposites

Research projects

Laser ablative and non-ablative treatment of polymers: approach to novel polymeric structures

(J. Pola, supported by GA ASCR, grant No. 104/04/2028)

Laser-induced ablative decomposition of various polymers was revealed as a very specific process useful to deposition of novel polymeric films and involving a multitude of yet unknown degradation steps in the solid phase. IR laser ablative degradation of poly(vinyl chloride) involves new decomposition paths leading to nanostructured polymeric films incorporating carbonaceous nano-fibers and nano-necklaces [Ref. 1]. IR laser ablative decomposition of poly(vinyl acetate) loaded with Fe and Cu particles was demonstrated as a feasible process for deposition of thin metal/polymer films with amorphous forms of metals embedded in and protected by polymeric matrix [Ref. 2]. IR laser ablative modification of poly(ethylene-co-acrylic acid) zinc salt was shown as a specific process remarkably different from conventional degradation, leading to enrichment of deposited films with Zn salt [Ref. 3]. Thermal degradation of poly(vinyl chloride-co-vinyl-acetate) and its laser derived analogue revealed that the degradation of the latter consists in accelerating effect of the intermediary conjugated C=C bonds and their crosslinking [Ref. 4]. IR laser-induced ablative decomposition of poly(vinyl acetate) was shown as a unique process allowing the control of products by irradiating conditions. Conversely to the conventional degradation allowing products with the initial O/Cl ratio, the laser-induced process affords deposition of polar cross-linked films in which the proportion of Cl and acetoxy groups is controlled by irradiation parameters [Ref. 5]. Laser ablative decomposition/deposition of poly(ethylene succinate) occurs as depolymerization/repolymerization process involving molecular ester

group interchange and a sequence of the C-C bond homolysis and recombination of the produced radicals [Ref. 6]. IR laser ablation of poly(ethylene terephthalate) yields insoluble polymeric films with two different – the initial and a –COOH - polar groups [Ref. 7]. IR laser ablative degradation of poly(vinyl phenyl ketone) was demonstrated as a process entirely different from conventional degradation and affording polar crosslinked films with less keto groups than in the initial polymer [Ref. 8].

Laser fabrication of Fe and γ -Fe₂O₃/polymer nanocomposites of superior thermal stability

(J. Pola, supported by NATO collaborative project, grant No. CLG980587)

Laser-assisted one-step procedure consisting in continuous-wave IR laser-induced and ethylene-sensitized co-pyrolysis of gaseous iron pentacarbonyl and hexamethyldisiloxane in argon was optimized for production of nano-magnetic Fe-based composites that were revealed to consist of Fe-based core and siloxane-based shell. The composites show superior thermal stability and sensing properties. [Ref. 19]

Laser initiated chemical vapour deposition of nanosulphides

(J. Pola, supported by Ministry of Education, Grant No. 1016/2006-32)

IR laser-induced co-thermolysis and UV laser-induced co-photolysis of two different progenitors to two different elements (metal and chalcogen) allows chemical vapour deposition of nanostructured metal chalcogenides (SnTe [Ref. 9] and germanium sulfides [Ref. 13]). Such laser-initiated chemistry is the first example of synthesis of inorganic compounds in the gas phase. Similar approach employing progenitors containing Se and Si atoms results in deposition of polyselenocarbosilane films in which SiSe, proven to exist in the gas phase, was not detected as a consequence of his high reactivity towards other intermediate products [Refs. 12, 18].

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 GA ASCR, Grant No. 400720619)

MW and GW UV laser-induced photolysis of several aromatic hydrocarbons and diacetylene 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. Heating of the carbon/silica/polyoxocarbosilane nanocomposite indicates a low-temperature formation of silicon carbide. [17]

Pyrolytic and photolytic approach for the deposition of novel Si/Ge/C materials

(V. Dřínek, supported by GA ASCR, grant No. A400720616)

The project deals with production of novel Si/Ge/C materials by means of laser CVD, ablative decomposition and MAPLE and pyrolytic techniques. The starting precursors are various polymeric, liquid and gaseous silagermanes with different Si/Ge/C ratio. Conventional pyrolysis and laser ablation of linear poly(germasilaethyne) were revealed to be different processes, the first yielding Si/Ge/C composite containing Ge nanoparticles and the other leading to extrusion of dimethylgermylene and deposition of poly(carbosilane). Low-fluence laser irradiation of poly(germasilaethyne) results in depletion of triple C-C bonds and crosslinking. Conventional pyrolysis of the crosslinked polymer affords polymeric material with increased Si/Ge ratio. [21]

Novel preparation and photocatalytic study of titania-based catalysts

(R. Fajgar, supported by NATO collaborative project, grant No. CBP.EAP.CLG.982078)

IR laser induced deposition of TiO₂ and Ti/O/Si films from two different precursors [titanium tetraisopropoxide and tetrakis(trimethylsiloxy)titanium] was studied. The films after annealing at 450°C revealed photocatalytic activity. Analysis of the prepared films confirmed formation of anatase with average particle size of about 40 nm. UV laser photolysis of the precursors in the gas phase affords deposition of thin and transparent amorphous films with very good adhesion to glass and quartz substrates. The same photolysis in the presence of oxygen was revealed to have explosive course. The deposits prepared cover reactor walls and TiO₂-anatase is formed directly.

Laser initiated chemical vapour deposition of nanosulphides

(J. Pola, supported by Agency of innovative enterprising AiP, Grant No. 7-2006-23)

IR laser-induced co-thermolysis of trisilane and thiirane (progenitors to silicon and sulphur elements) allows chemical vapour deposition of nanostructured SiS-containing polythiacarbosilane films. The SiS bodies in these nanocomposites are protected by the polymer for limited periods of time.

International co-operations

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

Chiba University, Chiba, Japan: Laser-induced production of novel Ge-incorporating polymers

Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of polycarbosilanes and silicon carbide

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

University of Crete, Heraklion, Greece: Laser and Cl atom - induced chemical vapour deposition of polycarbosilazanes

King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia: Reactive ablation for deposition of novel polymeric films

National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania: Laser-induced CVD of Fe/polymer nanocomposites

Visits abroad

J. Pola: National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan (6 weeks)

Visitors

L. Díaz, Institute of Structure of Materials, CSIC, Madrid, Spain

R. Tomovska, University of St. Cyril and Methodius, Skopje, Macedonia

J. Blazevska-Gilev, University of St. Cyril and Methodius, Skopje, Macedonia
L. Florescu, National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania

Publications

Original papers

1. Blazevska-Gilev J., Kupčik J., Šubrt J., Bastl Z., Vorlíček V., Galíková A., Spaseska D., Pola J.: IR Laser Ablation of Poly(vinyl chloride): Formation of Monomer and Deposition of Nanofibers of Chlorinated Polyhydrocarbon. *Polym. Degrad. Stabil.* 91(2), 213-220 (2006).
2. Blazevska-Gilev J., Kupčik J., Šubrt J., Bastl Z., Galíková A., Pola J.: IR Laser Ablative Decomposition of Poly(vinyl acetate) Loaded with Fe and Cu Particles. *Polym. Degrad. Stabil.* 91(9), 2241-2248 (2006).
3. Blazevska-Gilev J., Šubrt J., Bastl Z., Pola J.: IR Laser Ablative Modification of Poly(ethylene-co-acrylic acid) Zinc Salt. *Polym. Degrad. Stabil.* 91(12), 2834-2839 (2006).
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8. Morita H., Nozawa R., Bastl Z., Šubrt J., Pola J.: Photochemical Synthesis of Ultrafine Organosilicon Particles from Trimethyl(2-propynoxy)silane and Carbon Disulfide. *J. Photochem. Photobiol. A* 179(1-2), 142-148 (2006).
9. Pokorná D., Boháček J., Vorlíček V., Šubrt J., Bastl Z., Volnina E.A., Pola J.: IR laser Co-Pyrolysis of (CH₃)₂Te and (CH₃)₄Sn: Gas-Phase Formation and Deposition of Nanostructured SnTe. *J. Anal. Appl. Pyrolysis* 75(2), 65-68 (2006).
10. Pokorná D., Galíková A., Šubrt J., Blechta V., Pola J.: IR Laser Ablative Decomposition and Depolymerization/Repolymerization of Poly(ethylene succinate). *Polym. Degrad. Stabil.* 91(12), 3383-3389 (2006).
11. Pola J., Galíková A., Bastl Z., Šubrt J., Vacek K., Brus J., Ouchi A.: UV Laser Deposition of Nanostructured Si/C/O/N/H Precursor to Silicon Oxycarbonitride. *Appl. Organometal. Chem.* 20(10), 648-655 (2006).
12. Santos M., Diaz L., Urbanová M., Pokorná D., Bastl Z., Šubrt J., Pola J.: IR Laser-Induced Process for Chemical Vapor Deposition of Polyselenocarbosilane Films. *J. Anal. Appl. Pyrolysis* 76(1-2), 178-185 (2006).
13. Tomovska R., Vorlíček V., Boháček J., Šubrt J., Pola J.: UV Laser Co-Photolytic Approach to Gas-Phase Formation and Deposition of Nano-Sized Germanium Sulfides. *J. Photochem. Photobiol., A* 182(1), 107-111 (2006).
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15. Díaz L., Santos M., Pola J.: Gas-Phase Formation of SiSe in IR laser-co-decomposition of Dimethyl Selenide and 1,3-Disilacyclobutane. *J. Anal. Appl. Pyrolysis*, submitted.

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18. Santos M., Díaz L., Urbanová M., Bastl Z., Šubrt J., Pola J.: IR Laser-Induced Co-decomposition of Dimethyl Selenide and Trisilane: Gas-Phase Formation of SiSe and Chemical Vapor Deposition of Nanostructured H/Si/Se/C Polymers. *J. Photochem. Photobiol., A*, submitted.
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International conferences

22. Alexandrescu R., Morjan I., Dumitrache F., Gavrilă-Florescu L., Voicu I., Pola J., Vorlíček V., Maryško M., Bastl Z., Prodan G.: Structural and Magnetic Properties of Nanosized Iron-Polyoxocarbosilane Core-Shell Composites Prepared by Laser Pyrolysis. International Conference on Advanced Laser Technologies, Book of Abstracts, p. 1, Brasov, Romania, 08-12 September 2006.
23. Díaz L., Santos M., Urbanová M., Pola J.: Real Time Study of Photodissociation of Trisilane and Dimethylselenide Induced by IR Laser. XX Reunión Nacional de Espectroscopia (RNE) y IV Congreso Ibérico de Espectroscopia (CIE), Ciudad Real, Spain, 10-14 September 2006.
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25. Maryško M., Jiráček Z., Jiráčková Y., Knížek K., Pola J.: Experimental Investigation of the Cluster Glass Magnetism in Mixed FM-AFM Phases. International Conference on Magnetism, Abstracts, Kyoto, Japan, 20-25 August 2006.
26. Morjan I., Pola J., Alexandrescu R., Dumitrache F., Tomescu A., Opletal L., Chobot V., Soare I., Voicu I., Galíková A., Ciupina V., Bastl Z.: Newly Developed Fe-Fe₂O₃/Polyoxocarbosilane Core-Shell Nanocomposite Prepared by Laser Pyrolysis: Characterization and Sensing Properties. MRS-Materials Research Society Symposium, Proceedings, p. 0915-R03-05, San Francisco, USA, 17-21 March 2006.
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28. Tomescu A., Alexandrescu R., Morjan I., Dumitrache F., Albu L., Ciupina V., Bastl Z., Galíková A., Pola J.: Sensing Properties of a Novel Fe-Fe₂O₃/Polyoxocarbosilane Core-Shell Nanocomposite Powder Prepared by Laser Pyrolysis. Materials Science & Technology Conference, Nanomaterials: Materials and Processing for Functional Applications, San Antonio, USA, 12-16 March 2006.
29. Dřínek V., Vacek K.: Surface Point Defects in Silicon Related Nanopowders Produced by Pulsed Laser Ablation: IR Evidence of Peroxy Radical SiOO(.). 5th International Conference on Nanomaterials and Nanotechnologies NANO 06, Proceedings NANO 06 p.117, Brno, Czech Republic, 13-15 November 2006

Department of Analytical Chemistry

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Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

Applied research

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

Research projects

Advanced techniques for ^{29}Si NMR spectroscopy

(J. Schraml, supported by GA CR, grant No. 203/06/0738)

Two topics - ^{29}Si - ^{13}C spin-spin coupling constants and LC- ^{29}Si -NMR - are integrated under this project. The newly developed methods for measurements of the coupling constant will enable otherwise difficult line assignments [Ref. 5], the LC-NMR part will focus on industrially important silicones where it offers entirely new possibilities [Ref. 2].

Enzymatic catalysis in supercritical carbon dioxide

(Participation in the project supervised by H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry of the ASCR supported by the Ministry of Education, COST project D30.001)

Our participation is directed at LC-NMR identification of the products from enzymatic modifications of blackcurrant seed oil separated by supercritical carbon dioxide continuous-flow extraction. The aim is to develop an integrated production and product recovery process for the extraction from seed and lipase catalysis in supercritical CO_2 .

Reactivity of asymmetrically substituted epimino pyranoses

(J. Karban, supported by ICPF)

Nucleophilic aziridine ring cleavage of 2,3,4-trideoxy-2,3-tosyl/nosylepimino-1,6-anhydro- β -D-hexopyranoses was studied. The epimino derivatives of *ribo* configuration

afforded products of *trans*-diaxial cleavage whereas epimino derivatives of *lyxo* configuration gave products of both *trans*-diaxial and *trans*-diequatorial cleavage [Ref. 13]). Primary products of the cleavage often underwent a partial or complete halogen exchange (an analogy of the Finkelstein reaction).

International co-operations

Catholic University of Leuven, Leuven, Belgium: NMR in medicinal chemistry
Technical University Graz, Austria: ^{29}Si NMR

Teaching

J. Schraml: CU and ICT, course "NMR spectroscopy"

Publications

Original papers

1. Bártlová M., Bernášek P., Sýkora J., Sovová H.: HPLC in Reversed Phase Mode: Investigation of Kinetics of Blackcurrant Seed Oil Lipolysis in Supercritical Carbon Dioxide. *J. Chromatogr., B: Biomed. Appl.* 839(1-2), 80-84 (2006).
2. Blechta V., Sýkora J., Hetflejš J., Šabata S., Schraml J.: ^{29}Si NMR in LC-NMR Analysis of Silicones. *Magn. Reson. Chem.* 44(1), 7-10 (2006).
3. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus : Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.* 38(2), 121-131 (2006).
4. Pokorná D., Galíková A., Šubrt J., Blechta V., Pola J.: IR Laser Ablative Decomposition and Depolymerization/Repolymerization of Poly(ethylene succinate). *Polym. Degrad. Stabil.* 91(12), 3383-3389 (2006).
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7. Žáček P., Dransfeld A., Exner O., Schraml J.: ^{15}N NMR Chemical Shifts of Ring Substituted Benzonitriles. *Magn. Reson. Chem.* 44(12), 1073-1080 (2006).
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9. Čermák J., Žádný J., Krupková A., Lopatová K., Vlachová A., Nguyen Thi T.H., Šauliová J., Sýkora J., Císařová I.: Tetramethyl(perfluoroalkyl)cyclopentadienyl Rhodium(III) Complexes Containing Phosphorus and Nitrogen Monodentate Donors. Crystal Structure of $[(\text{h}5\text{-C}_5\text{Me}_4\text{C}_4\text{F}_9)\text{Rh}(\text{PPri}_3)\text{Cl}_2]$. *J. Organomet. Chem.*, submitted.
10. Pekárek V., Weber R., Grabic R., Šolcová O., Fišerová E., Šyc M., Karban J.: Matrix Effect on the De novo Synthesis of Polychlorinated Dibenzo-p-dioxins, Dibenzofurans, Biphenyls and Benzenes. *Chemosphere*, in press.

11. Šabata S., Blechta V., Karban J., Pleska A., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. Phosphorus, Sulfur and Silicon, submitted.
12. Šabata S., Blechta V., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. J. Organomet. Chem., submitted.

Chapters in books

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