

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 2005

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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 Drahoš
(since September 2005)	Jiří Smolík
Deputy Director (Business Administration)	Eva Melková
Scientific Secretary	Jan Linek
Scientific Board Chairman	Karel Aim

DEPARTMENTS

Department of Diffusion and Separation Processes (page 5)
E. Hála Laboratory of Thermodynamics (page 14)
Department of Catalysis and Reaction Engineering (page 23)
Department of Multiphase Reactors (page 32)
Department of New Processes in Chemistry and Biotechnology (page 41)
Environmental Process Engineering Laboratory (page 47)
Laboratory of Aerosol Chemistry and Physics (page 52)
Laboratory of Laser Chemistry (page 59)
Department of Analytical Chemistry (page 64)

STAFF

(31 December 2005)

Category	Number of Employees
Research	131
Technical	23
Administrative	17
Services	15

BUDGET 2005

(24 Kč ≈ 1 US\$, 30 Kč ≈ 1 EUR)

Resources	Million Kč
Institutional support based on Institutional Research Plan	84
Targeted support from Grant Agencies and R&D Programmes in the Czech Republic	22
Foreign R&D Funds and European Programmes	3
Contracts with industry	3
Total Resources	112

Expenses	Per cent of Total Resources
Personal expenses including mandatory insurance	58
Purchase of material	12
Purchase of services	7
Repairs and maintenance	7
Depreciation of fixed assets	7
Travel expenses	4
Energy, water, and fuels	3
Total other expenses	2

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. Sajfřtová, H. Sovová, P. Uchytíl, E. Volaufová
Part time: J. Procházka †, V. Staněk, H. Vychodilová
Technical staff: A. Kadlecová, D. Karfík, M. Koptová, D. Vlček
PhD students: K. Aleksieva, P. Bernášek, K. Fialová, 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 secondary industrial resources
- 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 research of electroorganic synthesis in electrochemical microreactor. An effort is focused on hydrodynamic study of two phase flow in narrow channel. The results of this research are a part of the research in several subtasks of the project. [Refs. 53-58]

Operation of counter-current columns in a dynamic state with periodic excursions beyond flooding points

(V. Jiříčný, supported by GA CR, grant No. 104/03/1558)

As a part of our basic research we have found that the dynamics of transition of the hydrodynamic regime towards flooding is different from that of recovery of the state existing prior to the flooding. On the basis of this finding the goal of this project is to study the possibilities of operating the counter-current packed bed column in the dynamic state forced by imposed changes of the flow rates of either liquid or gas with periodic excursions into the domain beyond the flooding point. [Refs. 1, 21, 60, 64, 65]

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

(V. Jiříčný, joint project with Institute of Chemical Technology, Prague 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. 28] and method of intensification [Refs. 2, 46, 49, 51 66, 67, 69] and safe control [Refs. 18, 39, 48, 72] 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. 65, 70].

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. [Ref. 68]

Enzymatic catalysis in supercritical carbon dioxide

(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry AS CR, 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 extractor [Refs. 31, 32]. The aim is to develop an integrated production and product recovery process for the extraction from seed and lipase catalysis in

supercritical CO₂. The extraction step was studied, partially in cooperation with Bulgarian and Macedonian colleagues, for different plants [Refs. 7, 11, 16, 23-26, 33, 45, 62, 63], and a generalized model for supercritical fluid extraction of plants was developed [Refs. 8, 29, 61].

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

(H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry AS CR, 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 ethanolysis of blackcurrant oil follows after its supercritical fluid extraction from the seed [Refs. 10, 30]. The aim of the project is to obtain variable and controlled α - to γ -linolenic acid ratios in the produced ethyl esters.

Relations between morphology and activity of polymer-supported catalysts

(K. Jeřábek, supported by ICPF)

Studies of the influence of the concentration acidic groups in ion exchangers adjusted by various methods demonstrated the inhomogeneity of the acid strength of the active centers of formally homogeneous chemical composition [Ref. 3] and differences in sensitivities of various reactions toward morphology of the polymer supports [Refs. 17, 50]. In cooperation with Italian colleagues from Padua University, Italy, we studied the metal nanoparticle catalysts supported in polymer gel networks. [Refs. 6, 14]

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 [Ref. 52], atomic force microscopy, and others.

Study of transport phenomena in polymeric membrane during pervaporation

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

Sorption in steady state of vapour permeation was studied and the model of toluene transport in polyethylene membrane during vapour permeation was proposed [Refs. 15, 40-44]. Diffusion coefficients of vapour permeating through polymer membranes were evaluated from dynamic permeation experiments. The mathematical model was developed, where the non-perfect step input concentration function is included in the description of the transport through a polymer. The influences of the upstream volume and the flow rate of permeating vapours on errors of the diffusion coefficient evaluation were discussed [Refs. 12, 13, 20, 37, 38]. The transport properties of dense film membranes (30-50 μm thick) based on cellulose myristate were studied for separation of toluene-ethanol, toluene-methanol or benzene-ethanol mixtures at 20-30 °C. Application of pervaporation method for separation of mixtures containing 10-80 mass % of aromatics provides membrane selectivity in relation to aromatic hydrocarbons. The values of the separation factor (2.1-36.3) increased and flux decreased with decreasing of toluene (benzene) content in feed composition [Ref. 59].

Ceramic materials with hierarchical porous structure for membrane separation technologies

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

Membrane technologies become an important alternative to classical ones. Ceramic membranes are important in high temperature processes. Project was stimulated by a requirement to decrease production costs of hierarchical porous structure of micro- and nano-filtration membranes. A prospective way to decrease these costs is to decrease the number of interlayers in membranes. Nanofiltration layers will be realized on the basis of zeolites Silikalit-1, NaA, NaY a DD3R. The ceramic support on the basis of α -alumina was prepared and its porous structures was studied by gas permeation method and compared with the results of mercury porosimetry. The conditions of vapour condensation in pores of Vycor glass membrane were studied and results were published. [Refs. 9, 27, 37, 38]

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, Republic of South Africa (5 weeks)
P. Izák: University of Lisboa, Portugal, and University of Rostock, Germany (1 year)
J. Ondráček: Technical University of Crete, Chania, Greece (7 months)

Visitors

M. Čársky, University of Durban, Republic of South Africa
J. Dudas, CSIR, Johannesburg, Republic of South Africa
J.W. Evans, University of California at Berkeley, USA
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. Akramov T., Stavárek P., Jiříčný V., Staněk V.: The Hydrodynamics of Counter-Current Packed Bed Exposed to Periodic Variations of Inlet Velocity - Analysis. *Ind. Eng. Chem. Res.* 44(24), 9931-9938 (2005).
2. Dudas J., Hanika J., Lepuru J., Barkhuysen M.: Thymol Hydrogenation in Bench Scale Trickle Bed Reactor. *Chem. Biochem. Eng. Q.* 19(3), 255-262 (2005).
3. Holub L., Jeřábek K.: Influence of Partial Neutralization on Catalytic Activity of Ion Exchange Resin. *J. Mol. Catal.* 231(1-2), 21-26 (2005).
4. Izák P., Mateus N.M.M., Afonso C.A.M., Crespo J.G.: Enhanced Esterification Conversion in a Room Temperature Ionic Liquid by Integrated Water Removal with Pervaporation. *Sep. Purif. Technol.* 41(2), 141-145 (2005).
5. Jeřábek K.: Polymers and Organic Chemistry. *Chem. Int.* 27(1), 29 (2005).
6. Pozzar F., Sassi A., Pace G., Lora S., D'Archivio A.A., Jeřábek K., Grassi A., Corain B.: Gel-Type Polyacrylic Resins Cross-Linked with Trimethylolpropanetriacrylate: The Issue of Their Nanostructure and Molecular Accessibility Unveiled with a Combination of Inverse Steric Exclusion Chromatography (ISEC), and ESR and CP-MAS ¹³C NMR Spectroscopy. *Chem. Eur. J.* 11(24), 7395-7404 (2005).
7. Sajfritová M., Sovová H., Opletal L., Bártlová M.: Near-Critical Extraction of β -Sitosterol and Scopoletin from Stinging Nettle Roots. *J. Supercrit. Fluids* 35(2), 111-118 (2005).
8. Sovová H.: Mathematical Model for Supercritical Fluid Extraction of Natural Products and Extraction Curve Evaluation. *J. Supercrit. Fluids* 33(1), 35-52 (2005).

9. Yang J., Čermáková J., Uchytíl P., Hamel CH., Seidel-Morgenstern A.: Gas Phase Transport, Adsorption and Surface Diffusion in Porous Glass Membrane. *Catal. Today* 104(2-4), 344-351 (2005).
10. 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.*, submitted.
11. Bocevska M., Sovová H.: Supercritical CO₂ Extraction of Essential Oil from Yarrow. *J. Supercrit. Fluids*, submitted.
12. 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.*, in press.
13. 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.*, in press.
14. D'Archivio A.A., Tauro L., Galantini L., Panatta A., Tettamanti E., Giammatteo M., Jeřábek K., Corain B.: On the Peculiar Micro- and Nanomorphology of the Catalytically Useful Commercial Resin Poly-4-vinylpyridine-divinylbenzene. *React. Funct. Polym.*, submitted.
15. 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.*, in press.
16. 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.*, submitted.
17. Hanková L., Holub L., Jeřábek K.: Relation between Functionalization Degree and Activity of Strongly Acidic Polymer Supported Catalysts. *React. Funct. Polym.*, in press.
18. Kaštanek F., Hanika J.: Úloha chemického inženýrství ve zvyšování bezpečnosti chemických výrob. (Czech) The Role of Chemical Engineering in Chemical Process Safety. *Chem. Listy*, 100, 150-155 (2006).
19. Kaštanek F., Maléterová Y., Kaštanek P., Rott J., Jiříčný V., Jirátová K.: Complex Treatment of Soils, Waste Water and Groundwater Contaminated by Halogenated Organic Compounds. *Desalination*, in press.
20. 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.
21. 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. *Ind. Eng. Chem. Res.*, submitted.
22. Procházka J., Heyberger A., Volaufová E.: Effect of Diluents on Sulfuric Acid Extraction with Trialkylamine. *AIChE J.*, submitted.
23. Sovová H., Aleksovski S.: Mathematical Model for Hydrodistillation of Essential Oils. *Chem. Eng. Sci.*, submitted.
24. Sovová H., Aleksovski S., Bocevska M., Stateva R.P.: Supercritical Fluid Extraction of Essential Oils - Results of Joint Research. *Chem. Industry Chem. Eng. Q.*, submitted.
25. Sovová H., Opletal L., Bártlová M., Sajfřtová M., Křenková M.: Supercritical Fluid Extraction of Lignans from Caulomas and Leaves of *Schizandra Chinensis*. *J. Supercrit. Fluids*, submitted.
26. Sovová H., Stateva R.P., Galushko A.A.: High Pressure Equilibrium of Menthol + CO₂. *J. Supercrit. Fluids*, submitted.
27. Uchytíl P., Petříčkovič R., Seidel-Morgenstern A.: Study of Capillary Condensation of Butane in Vycor Membrane. *J. Membr. Sci.*, 264, 27-36 (2005).

Review papers

28. Silveston P. L., Hanika J.: Periodic Operation of Three Phase Catalytic Reactors, *Can. J. Chem. Eng.*, 82(6), 1105-1142 (2004), published (2005).

Chapters in books

29. Sovová H.: Modeling of Supercritical Fluid Extraction from Plant Materials. In: Engineering Technologies and Processing of Functional Foods. (Shi, J. - King, J., Ed.), CRC Press, in press.

Conferences

30. 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. 4th International Symposium on Separations in the BioSciences (SBS'05), Symposium Program & Abstracts, p. 76, Utrecht, Netherlands, 18-21 September 2005.
31. Bernášek P., Sovová H.: Enzymová hydrolyza v průtočném reaktoru. (Czech) Enzyme Catalysed Hydrolysis in a Continuous-Flow Reactor. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 213, Srní, Šumava, Czech Republic, 17-20 October 2005.
32. Bernášek P., Zarevúcka M., Sovová H., Bártlová M., Stránský K., Cvačka J.: Blackcurrant Oil Hydrolysis in SC-CO₂: Experiment and Model. 10th European Meeting on Supercritical Fluids, Book of Abstracts, p. N15, Colmar, France, 12-14 December 2005.
33. Bocevska M., Sovová H.: Extraction of Essential Oil from Yarrow with Supercritical CO₂: Effect on Antiradical Activity. 1st South East European Congress of Chemical Engineering, Book of Abstracts, p. 102, Belgrade, 25-28 September 2005.
34. Břenková L., Bělohav Z., Durdil P., Hanika J., Kalčíková J., Tomášek V.: Matematické modelování procesu mokré granulace. (Czech) Mathematical Modeling of Wet Granulation Process. 32. Technologické dny, Bratislava, Slovakia, 08-09 September 2005, (Farmaceutický obzor 74(8), 221, 2005).
35. Břenková L., Bělohav Z., Durdil P., Hanika J., Kalčíková J., Tomášek V.: Optimalizace procesu mokré granulace využitím fuzzy logiky. (Czech) Wet Granulation Process Optimization Using Fuzzy Logic. 57. zjazd chemických společností, ChemZi 1/1 2005, p. 116, Tatranské Matliare, Slovakia, 04-08 September 2005.
36. Břenková L., Bělohav Z., Durdil P., Hanika J., Kalčíková J., Tomášek V.: Fuzzy modelování procesu mokré granulace léčiv. (Czech) Fuzzy Modeling of Drug Wet Granulation Process. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 87, Srní, Šumava, Czech Republic, 17-20 October 2005.
37. Čermáková J., Fialová K., Petříčkovič R., Kudrna V., Uchytíl P.: Význam návrhu cely z hlediska přesnosti stanovení difusního koeficientu z permeačních experimentů. (Czech) 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 40, Srní, Šumava, Czech Republic, 17-20 October 2005.
38. Čermáková J., Fialová K., Petříčkovič R., Kudrna V., Uchytíl P.: Effect of Input Non-perfect Step Concentration Function on Diffusion Coefficient Evaluation. Membrane Science and Technology Conference of Visegrad Countries PERMEA 2005, Book of Abstracts, p. 167, Polanica Zdrój, Poland, 18-22 September 2005.
39. Dudas J., Hanika J., Barkhuysen M.: Hydrogenation of Thymol and Racemisation of Menthol Mixture in Trickle Bed Reactor (TBR): Reactor Design, Scale Up and Safe Operation. 5th International Symposium on Catalysis in Multiphase Reactor and 4th International Symposium on Multifunctional Reactors, Book of Extended Abstracts, p. 169-170, Portorož-Portorose, Slovenia, 15-18 June 2005.
40. Fialová K., Petříčkovič R., Uchytíl P.: Transport Mechanism in Polyethylene Membrane during Vapor Permeation of Propan-1-ol and Toluene. Application of Nanotechnologies for Separation and Recovery of Volatile Organic Compounds from Waste Air Streams, Proceedings, p. 45-50, Istanbul, Turkey, 30 May - 01 June 2005.
41. Fialová K., Petříčkovič R., Uchytíl P.: Transport Phenomena through Unswollen and Swollen Polymeric Membrane. 5 Congreso Iberoamericano de Ciencia y Tecnología de Membranas, Book of Abstracts, p. 109, Valencia, Spain, 06-08 July 2005.
42. Fialová K., Petříčkovič R., Uchytíl P.: New Type of Apparatus for Sorption Measurements during Vapor Permeation in Polymeric Membrane. International Congress on Membranes and

- Membrane Processes 2005, Program and Abstracts, p. 186, Seoul, South Korea, 21-26 August 2005.
43. Fialová K., Petříčkovič R., Uchytíl P.: Využití sorpce měřené v ustáleném tvaru permeace par k popisu transportu látek v polymerní membráně. (Czech) Description of Vapor Transport in Polymeric Membranes Using the Sorption Data in Steady State Vapor Permeation Process. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 43, Srní, Šumava, Czech Republic, 17-20 October 2005.
 44. Fialová K., Uchytíl P., Petříčkovič R.: Study of Transport through Polymeric Membrane during Vapor Permeation - Membrane Swelling. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 281, Tatranské Matliare, Slovakia, 23-27 May 2005.
 45. Galushko A.A., Sovová H., Stateva R.P.: Solubility of Menthol in Pressurised Carbon Dioxide – Experimental Data and Thermodynamic Modelling. 1st South East European Congress of Chemical Engineering, Book of Abstracts, p. 101, Belgrade, 25-28 September 2005.
 46. Hanika J.: Dynamické řízení hydrogenačního reaktoru se zkrápěnou vrstvou katalyzátoru. (Czech) Dynamic Control of Hydrogenation Process in Trickle Bed Reactor. 14. Konference APROCHEM 2005. Chemické technologie, Petrochemie, Polymery, Ropa, Paliva, Sborník přednášek, p. 127-132, Milovy, Czech Republic, 24-26 October 2005.
 47. Hanika J.: Applied Research in the Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic (ASCR), Prague. 57. zjazd chemických společností, ChemZi 1/1 2005, p. 121, Tatranské Matliare, Slovakia, 04-08 September 2005.
 48. Hanika J., Jiříčný V., Kolena J., Lederer J., Stavárek P., Šimek J., Tukač V.: Intenzifikace, bezpečné řízení a provozování průmyslově zkrápěných reaktorů. (Czech) Intensification, Safety Control and Operation of Trickle Bed Reactors in Industrial Practice. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 118, Srní, Šumava, Czech Republic, 17-20 October 2005.
 49. Hanika J., Skořepová J., Karnetová-Houserová P.: Dynamic Operation of Trickle Bed Reactors: CSTRs Cascade Model. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 224, Tatranské Matliare, Slovakia, 23-27 May 2005.
 50. Hanková L., Holub L., Jeřábek K.: Relation between Functionalization Degree and Activity of Strongly Acidic Polymer Supported Catalysts. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 168, Tatranské Matliare, Slovakia, 23-27 May 2005.
 51. Chyba V., Tukač V., Hanika J., Šimíčková M., Sazanov Z.: Kinetika hydrogenace styrénu a dicyklopentadienu na palladiovém katalyzátoru. (Czech) Kinetics of Styrene and Dicyclopentadiene Hydrogenations on Pd Catalyst. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 122, Srní, Šumava, Czech Republic, 17-20 October 2005.
 52. Jeřábek K.: Morphology of Functional Polymers and Their Application Properties. 7th International Symposium on the Characterisation of Porous Solids COPS VII, Abstracts, p. 31, Aix en Provence, France, 25-28 May 2005.
 53. Křišťál J., Havlica J., Jiříčný V.: Porovnání 2D a 3D simulací proudění v mikroreaktoru. (Czech) 2D and 3D CFP Flow Simulations in Micro Reactor - Comparison. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 230, Srní, Šumava, Czech Republic, 17-20 October 2005.
 54. Křišťál J., Havlica J., Jiříčný V.: Simulace proudění v reaktoru s úzkou štěrbinou. (Czech) CFD Flow Simulation in Narrow Channel. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 46, Srní, Šumava, Czech Republic, 17-20 October 2005.
 55. Křišťál J., Havlica J., Jiříčný V.: Experimental Study of Bubbly Flow in a Thin-Gap Microreactor. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.11., Strasbourg, France, 21-24 August 2005.
 56. Křišťál J., Havlica J., Jiříčný V.: Numerical Simulation of Single Bubble Rise in a Thin-Gap Microreactor. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.12., Strasbourg, France, 21-24 August 2005.
 57. Křišťál J., Havlica J., Jiříčný V.: CFD Simulation of Gas-Liquid Flow in Narrow Channel. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 40, Tatranské Matliare, Slovakia, 23-27 May 2005.

58. Křišťál J., Havlica J., Jiříčný V.: CFD Simulation of Gas-Liquid Flow in Thin-Gap Channel. 11th Workshop on Two-Phase Flow Predictions, Book of Abstracts, p. 1, Merseburg, Germany, 05-08 April 2005.
59. Kuznetsov Yu.P., Khripunov A.K., Kruchinina E.V., Fialová K., Uchytíl P.: Cellulose Myristate Based Membrane for Separation of Aromatic Hydrocarbons and Aliphatic Alcohols. 5th International Symposium Molecular Mobility and Order in Polymer Systems, Book of Abstracts, St. Petersburg, Russia, 20-24 June 2005.
60. Ondráček J., Jiříčný V.: Hydrodynamic Behaviour of Counter - Current Bubble Bed Formed above the Packed Bed. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 43, Tatranské Matliare, Slovakia, 23-27 May 2005.
61. Sovová H.: Průmyslová extrakce z rostlin superkritickým CO₂ - praxe a teorie. (Czech) Large-Scale Supercritical Fluid Extraction from Plants – Practice and Theory. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 151, Srní, Šumava, Czech Republic, 17-20 October 2005.
62. Sovová H., Aleksovski S., Bocevska M., Stateva R.P.: Supercritical Fluid Extraction of Essential Oils - Results of Joint Research. 1st South East European Congress of Chemical Engineering, Book of Abstracts, p. 73, Belgrade, 25-28 September 2005.
63. Sovová H., Sajfritová M.: Experiments, Modelling and Scale-Up for Supercritical Extraction from Plants. 10th European Meeting on Supercritical Fluids, p. N4, Colmar, France, 12-14 December 2005.
64. Stavárek P., Ondráček J., Jiříčný V., Staněk V.: Hydrodynamic Behavior of Counter-Current Packed Beds in the Proximity of the Flooding Point Oscillating Inlet Velocities. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 133, Tatranské Matliare, Slovakia, 23-27 May 2005.
65. Stavárek P., Vychodilová H., Staněk V., Jiříčný V.: Charakteristika dvoufázového pulzního toku kapalina - plyn vrstvou zrnitého materiálu. (Czech) Characteristics of Two-Phase Gas-Liquid Pulsing Flow in Trickle Bed. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 45, Srní, Šumava, Czech Republic, 17-20 October 2005.
66. Šimíčková M., Tukač V., Chyba V., Lederer J., Kolena J., Šimek J., Hanika J.: Hydrogenace styrenu v pilotním zkrápěném reaktoru. (Czech) Styrene Hydrogenation in Pilot Trickle Bed Reactor. 57. zjazd chemických společností, ChemZi 1/1 2005, p. 117 (6P10), Tatranské Matliare, Slovakia, 04-08 September 2005.
67. Šimíčková M., Tukač V., Chyba V., Lederer J., Kolena J., Šimek J., Hanika J.: Styrene and Dicyclopentadiene Hydrogenation in Pilot Trickle-Bed Reactor. XXXVII Symposium on Catalysis, Book of Abstracts, p. 48, Prague, Czech Republic, 07-08 November 2005.
68. Tříška J., Heyberger A., Krtička M., Milichovský M., Růžičková K.: Tall Soap - Inconvenient Waste or Prospective Raw Material?. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 274, Tatranské Matliare, Slovakia, 23-27 May 2005.
69. Tukač V., Chyba V., Šimíčková M., Lederer J., Kolena J., Šimek J., Hanika J.: Přenos měřítka při hydrogenaci styrenu a dicyklopentadienu ve zkrápěném reaktoru. (Czech) Scale Up of Styrene and Dicyclopentadiene Hydrogenation in Trickle Bed Reactor. 14. Konference APROCHEM 2005. Chemické technologie, Petrochemie, Polymery, Ropa, Paliva, Sborník přednášek, p. 119-126, Milovy, Czech Republic, 24-26 October 2005.
70. Tukač V., Šimíčková M., Chyba V., Lederer J., Kolena J., Šimek J., Hanika J.: Steady-State and Periodic Behavior of Trickle-Bed Reactor. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 294, Tatranské Matliare, Slovakia, 23-27 May 2005.
71. Tukač V., Šimíčková M., Chyba V., Lederer J., Kolena J., Šimek J., Hanika J.: Dynamic Behavior of Trickle-Bed Reactor. 5th International Symposium on Catalysis in Multiphase Reactor and 4th International Symposium on Multifunctional Reactors, Book of Extended Abstracts, p. 87-88, Portorož-Portorose, Slovenia, 15-18 June 2005.
72. Hanika J.: Jsou chemické procesy nebezpečné?, Are Chemical Processes dangerous?, 2. Konference Bezpečnost v chemickém průmyslu, Ústí n.L., Czech Republic, 19-20 September 2005.

E. Hála Laboratory of Thermodynamics

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

Fields of research

- Determination of fluid phase equilibrium data at low, normal, and high pressures
- Experimental determination and molecular modelling of phase equilibria in systems with chemical reaction
- State and phase behaviour of liquids at superambient conditions (up to very high pressures)
- Thermodynamic modelling and processing of thermodynamic data
- Development of equations of state based on molecular theory
- Perturbation theories and molecular simulations for simple interaction potentials
- Molecular simulations and perturbation theories for model fluids and fluid mixtures
- Application of statistical–mechanical models to real fluids
- Molecular modelling of supercritical CO₂ + surfactant systems
- Theory of polar compounds
- Systems of associated fluids studied by statistical mechanics and simple models
- Hydrophobic interactions
- Molecular simulations of chemically reacting systems in nanoporous materials

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)

Measurements of phase equilibria in binary carbon dioxide + methanol, + ethanol, + 1-propanol, and + 2-propanol systems over extended ranges of conditions were completed. State behaviour of liquid octane + 1-chlorohexane mixtures at pressures up to 40 MPa was

also determined experimentally. Research continued on the variants of a newly developed perturbed equation of state for real methanol based on the molecular-level primitive model of association as well as on extending the approach to describe fluid phase equilibria in binary methanol + carbon dioxide mixtures. [Refs. 18, 22, 23, 41]

State behaviour of liquids and liquid mixtures

(J. Linek, supported by ICPF, project No. 2901)

Excess volumes determination in the systems of acetophenone with benzene, or toluene, or 1,3-xylene, or 1,3,5-trimethylbenzene and propiophenone with benzene, or toluene, or ethylbenzene, or butylbenzene at 298.15 K and 328.15 K and at atmospheric pressure was carried out. Afterwards, the P–V–T behaviour (toluene + propiophenone) was measured along five isotherms between 298.15 K and 328.15 K and at pressures up to 40 MPa. In addition to it, the density of propiophenone below its melting temperature was estimated both from the propiophenone density measurements at higher temperatures and from the correlation of excess volumes of (toluene + propiophenone) determined at temperatures below the propiophenone melting temperature. [Refs. 4, 5, 6, 17, 34, 35]

Prediction of solubility for large molecules in solvents by parallelized molecular simulation method

(M. Lísal, supported by GA ASCR, grant No. A4072309)

For studying electrolyte solution systems a new molecular-level simulation technique, the Expanded-Ensemble Osmotic Molecular Dynamics (EEOMD) method, was developed. The method performs simulations at fixed number of solvent molecules, pressure, temperature and overall electrolyte chemical potential and combines elements of constant pressure-constant temperature molecular dynamics and of expanded-ensemble grand canonical Monte Carlo. The method was tested for a model of NaCl in water at ambient conditions. First the chemical potential of NaCl in water was determined by the thermodynamic integration technique and by the expanded-ensemble method. Then the EEOMD simulations for different specified values of the overall NaCl chemical potential were carried out and the concentration of ions resulting from the simulations was measured. Both computations gave consistent results, validating so the EEOMD methodology. [Refs. 3, 33, 38, 39]

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

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

Behavior of chemically reacting fluids in nanoporous materials has been studied by molecular-level 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. Main efforts have been concentrated on the incorporation of realistic mass transport mechanisms into models of confined chemical reactions. The determination of the properties of nanoreactor systems should facilitate the implementation of nanoscale chemical devices. Several novel simulation methodologies have been developed to calculate the properties of chemically reacting fluids in nanoporous materials. [Refs. 2, 36, 37, 40, 50, 51]

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

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

New methods and algorithms for computer modelling and molecular simulations in geochemistry (particularly for geological fluid systems at extreme state conditions) have been under development. The main lines of research have been (1) state and phase behavior of

geological fluids at high temperatures and high pressures, and (2) physico-chemical properties of geological fluid systems at porous media. To this end, molecular simulation methodologies for high-density chemically-reacting fluid systems both in bulk and in confinement have been developed and tested. [Refs. 2, 11, 49]

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)

Methodology to construct primitive models for any given realistic Hamiltonian was completed [Refs. 1, 8]. The construction of the models was then followed by investigations of their thermodynamic properties and their theoretical description by means of the thermodynamic perturbation theory [Refs. 13, 14, 30, 31, 32, 44, 45, 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 deals with the development of new methods and algorithms for computer modelling and molecular simulations in material research for utilization of nanomaterials as nanoreactors and for materials with complex surface and/or bulk structure. In particular we have aimed at describing (1) morphological properties of materials and their relation to other physico-chemical properties, and (2) physico-chemical processes at or near the surface. Progress in developing the molecular simulation methodology for chemically reacting systems in nanopores and morphological analysis methodology for optimization of the laser welding technology has been achieved. [Refs. 7, 12, 46, 52]

Intermolecular interactions and associated phase diagrams of binary fluid mixtures

(I. Nezbeda, supported by MEYS, project Kontakt No. 2005-14)

The research has been focused on linking various types of intermolecular interactions to the possible occurrence of general phase behavior of fluid binary mixtures. Models of particular classes of intermolecular interactions amenable to a theoretical treatment have been used to get a thermodynamic model from which the complete phase behavior can be derived. [Refs. 21, 43]

Phase equilibria of complex fluid systems by means of fully parallelized Monte Carlo simulations

(I. Nezbeda, supported by ASCR, based on AS CR – CNRS agreement)

The research aims at improving phase equilibrium calculations in the cases when existing algorithms require too extensive computer time (several weeks) to consider thorough studies. Two examples considered were first the simulation of gas solubility in polymer melts, second the liquid-liquid equilibria at temperatures significantly lower than the normal boiling point. The selected approach consisted in using more efficiently the power of parallel computers. The clusters of several tens of PC processors under Linux provide indeed an important capacity at moderate cost, but the Monte Carlo methods do not use them as systematically as molecular dynamics. [Ref. 42]

Theory and molecular simulation of electric double-layer at solid-liquid surface

(M. Předota, supported by GA CR, grant No. 203/03/P083)

Molecular dynamics simulations were conducted to characterize the microstructure of the (110) rutile–aqueous electrolyte interface. In addition to structural characterization of the

interface (adsorption sites, structure of water at interface, surface hydroxylation), the dynamical properties of the aqueous solution were obtained. These include inhomogeneous diffusivity of water at the interface and inhomogeneous viscosity profile. Particularly the determination of the latter is a unique result, with special relevance to interpretation of electrophoretic data and to the modelling of the interface. This work presents the very first determination of space-dependent viscosity of a molecular fluid (water) by using computer simulations. A generalization of the method has also been devised and implemented. The applications of the study are in colloid chemistry (stability of colloid solutions), biochemistry (cell membranes) and geoenvironmental engineering. [Refs. 19, 47, 55]

State behaviour and phase equilibria in fluid systems

(I. Wichterle, supported by GA CR, grant No. 104/03/1555)

Systematic experimental determination of vapour–liquid equilibria has been conducted in binary and ternary systems composed of compounds containing selected structural groups (alkyl, hydroxyl, etheric, and ketonic) extending so the base for improving the group contribution methods. The data were supplemented by the measurement of molar excess volumes. New apparatus for liquid–liquid equilibrium investigations was constructed and data for systems containing ionic liquids were determined. A robust method has been elaborated which uses new algorithms eliminating solutions at local extremes for correlation of high-pressure data, and a new general computer program for vapour–liquid equilibrium data correlation has been developed. [Refs. 9, 10, 15, 16, 26–28, 34, 35]

Phase equilibria in reacting systems

(I. Wichterle, supported by GA CR, grant No. 203/03/1588)

Experimental determinations of phase equilibria have been carried out on model system with transesterification reaction, namely the quaternary ethanol + propyl acetate \leftrightarrow propanol + ethyl acetate system at isothermal conditions. On the theoretical side, the direct molecular simulation of a general reaction based on the Reaction Ensemble Monte Carlo (REMC) method has been further elaborated, modified, and applied to ammonia synthesis in flow reactor. [Refs. 2, 24, 25, 40, 53]

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

(J. Drahoš, I. Wichterle, supported by EU 5th RTD 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 lines of research were pursued: (a) Gas-liquid equilibria were determined at sub- and supercritical conditions in carbon dioxide + alcohol systems [Refs. 22, 23] and in the carbon dioxide + 1-chloropropane system; (b) 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 Diffusion and Separation Processes, Refs. 11, 23, 24, 33, 62]; (c) Simulation study of the thermodynamic properties of water-methanol mixtures; (d) Determination of vapour-liquid equilibrium and the solubility of impurities in industrial-grade liquid carbon dioxide; (e) The flow over a backward-facing step by measuring the instantaneous wall shear rate in the channel spanwise centerline; (f) Volumetric oxygen mass transfer coefficient in the bubble

column using dynamic pressure-step method [see Department of Multiphase reactors, Refs. 2, 5, 13, 20-22, 31].

International co-operations

DICAMP, University of Trieste, Italy: Phase equilibria for supercritical fluid technology
Technical University Vienna, Austria: Colloids and theory of fluids
Universite 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
Universitat Rovira i Virgili, Tarragona, Spain: Molecular-based studies of chemically reacting systems in nanoporous materials
Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania: Measurement and prediction of vapour-liquid equilibrium data
ITODYS, University of Paris VII, France: Vapour-liquid equilibrium bibliographic database; Phase equilibria in selected systems
Oak Ridge Natl. Laboratory, Oak Ridge, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems

Visits abroad

M. Lísal: University of Ontario Institute of Technology, Oshawa, ON, Canada (1 month)
I. Nezbeda: University of Ontario Institute of Technology, Oshawa, ON, Canada (1 month)
L. Vlček: Vanderbilt University, Nashville, TN, USA (12 months)

Visitors

M. Fermeglia, University of Trieste, Italy
S. Figuerola, University of Ontario, Institute of Technology, Oshawa, ON, Canada (1 month)
K. Fuchizaki, Department of Physics, Ehime University, Japan (1 month)
D. Gongalez-Salgado, University of Vigo, Vigo, Spain (3 months)
B. Rousseau, Université de Paris Sud, Orsay, France
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", "Numerical mathematics II"
I. Nezbeda: J. E. Purkyně University, Ústí n. L., course "Molecular theory of matter"

- I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"
- I. Nezbeda: J. E. Purkyně University, Ústí n. L., course "Statistical physics I"
- 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, course "Lectures from physics oriented to particle and nuclear physics"
- M. Předota: University of South Bohemia, Č. Budějovice, course "Selected lectures from physics"

Publications

Original papers

1. Chialvo A.A., Kettler M., Nezbeda I.: Effect of the Range of Interactions on the Properties of Fluids. 2. Structure and Phase Behavior of Acetonitrile, Hydrogen Fluoride, and Formic Acid. *J. Phys. Chem. B* 109, 9736-9750 (2005).
2. Lísal M., Bendová M., Smith W.R.: Monte Carlo Adiabatic Simulation of Equilibrium Reacting Systems: The Ammonia Synthesis Reaction. *Fluid Phase Equilib.* 235(1), 50-57 (2005).
3. Lísal M., Smith W.R., Kolafa J.: Molecular Simulations of Aqueous Electrolyte Solubility: 1. The Expanded-Ensemble Osmotic Molecular Dynamics Method for the Solution Phase. *J. Phys. Chem. B* 109, 12956-12965 (2005).
4. Morávková L., Linek J.: Excess Molar Volumes of (Propiophenone + Benzene, or Toluene, or Ethylbenzene, or Butylbenzene) at Temperatures 298.15 K and 328.15 K. *J. Chem. Thermodyn.* 37(9), 1023-1028 (2005).
5. Morávková L., Linek J.: Excess Molar Volumes of (Acetophenone + Benzene, or Toluene, or 1,3-Xylene, or 1,3,5-Trimethylbenzene) at Temperatures 298.15 K and 328.15 K. *J. Chem. Thermodyn.* 37(8), 814-819 (2005).
6. Morávková L., Wagner Z., Linek J.: (P, Vm, T) Measurements of (Toluene + Propiophenone) at Temperatures from 298.15 K to 328.15 K and at Pressures Up to 40 MPa. *J. Chem. Thermodyn.* 37(7), 658-666 (2005).
7. Moučka F., Nezbeda I.: Detection and Characterization of Structural Changes in the Hard-Disk Fluid Near Freezing/Melting Conditions. *Phys. Rev. Lett.* 94, 406011-406013 (2005).
8. Nezbeda I.: Towards a Unified View of Fluids. *Mol. Phys.* 103(1), 59-76 (2005).
9. Psutka Š., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Propanol, Diisopropyl Ether and 4-Methyl-2-Pentanone. *Fluid Phase Equilib.* 235(1), 58-63 (2005).
10. Psutka Š., Wichterle I.: Vapor-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Methylpentane, 3-Methyl-2-Butanone and 3-Methyl-2-Butanol. *J. Chem. Eng. Data* 50(4), 1338-1342 (2005).
11. Slovák J., Tanaka H.: Computer Simulation Study of Metastable Ice VII and Amorphous Phases Obtained by Its Melting. *J. Chem. Phys.* 122, 2045121-2045126 (2005).
12. Trokhymchuk A., Nezbeda I., Jirsák J., Henderson D.: Hard Sphere Radial Distribution Function Again. *J. Chem. Phys.* 123(2), 24501-24510 (2005).
13. Vlček L., Nezbeda I.: From Realistic to Simple Models of Fluids III. Primitive Models of Carbon Dioxide, Hydrogen Sulphide, and Acetone, and Their Properties. *Mol. Phys.* 103(14), 1905-1915 (2005).
14. Vlček L., Nezbeda I.: Potential of Mean Force between Ions Infinitely Diluted Simple Short-Range Models of Aqueous Electrolytes. *Condensed Matter Phys.* 8(2), 261-270 (2005).

15. Wichterle I.: "Secrets" of High Pressure Phase Equilibrium Experiment. *Kemija u Industriji* 54(11), 477-479 (2005).
16. 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.*, submitted.
17. Morávková L., Linek J.: Excess Molar Volumes of (Propiophenone + Toluene) and Estimated Density of Liquid Propiophenone below Its Melting Temperature. *J. Chem. Thermodyn.*, in press.
18. 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.*, in press.
19. Předota, M., Cummings, P. T., Wesolowski, D. J.: Electric Double Layer at the Rutile (110) Surface. 3. Inhomogeneous Viscosity Measurement by Computer Simulations. *J. Phys. Chem. B*, submitted.

Books and monographs

20. Linek J.: Annual Report 2004. 65 pp., Institute of Chemical Process Fundamentals AS CR, Prague 2005.

Chapters in books

21. Nezbeda I., Kolafa J.: Towards the Role of the Range of Intermolecular Interactions in Fluids. In: *Ionic Soft Matter: Modern Trends in Theory and Applications*. (Henderson, D. - Holovko, M. - Trokhymchuk, A., Ed.), pp. 83-108, Springer, Dordrecht 2005.

Conferences

22. Aim K., Babič A.: Thermodynamics of Phase Equilibria in Binary Carbon Dioxide + Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol Systems. *Thermodynamics 2005, Book of Abstracts*, p. 137, Sesimbra, Portugal, 06-08 April 2005.
23. Aim K., Babič A., Nezbeda I.: Systematic Treatment of Vapor-Liquid Equilibria in Carbon Dioxide + Alkanol Systems at Elevated Temperatures and Pressures. *10th Mediterranean Congress of Chemical Engineering, Abstracts*, p. 173, Barcelona, Spain, 15-18 November 2005.
24. Aim K., Wichterle I.: Vapor-Liquid Equilibrium Combined with Transesterification Reaction in the Quaternary Ethanol + Propyl Ethanoate + Propanol + Ethyl Ethanoate System. *10th Mediterranean Congress of Chemical Engineering, Abstracts*, p. 174, Barcelona, Spain, 15-18 November 2005.
25. Aim K., Wichterle I.: Isothermal Vapor-Liquid Equilibrium with Chemical Reaction in the Quaternary Water + Methanol + Acetic Acid + Methyl Acetate System. *Thermodynamics 2005, Book of Abstracts*, p. 136, Sesimbra, Portugal, 06-08 April 2005.
26. Barhala A., Dragoescu D., Teodorescu M., Wichterle I.: Vapor-Liquid Equilibria and Excess Gibbs Energies of Cyclopentanone + Chloroalkane Binary Mixtures. *Romanian International Conference on Chemistry and Chemical Engineering - RICCE XIV, Proceedings*, p. 25-34 (S03), Bucuresti, Romania, 22-24 September 2005.
27. Bendová M.: Liquid Phase Behaviour in Binary System 1-Butyl-3-methylimidazolium Hexafluorophosphate + Water by the Volumetric Method. *European/Japanese Molecular Liquids Group Annual Meeting, Praha, Czech Republic*, 04-08 September 2005.
28. Bendová M., Wichterle I.: Liquid-Liquid Equilibrium in Binary Systems 1-Butyl-3-methylimidazolium Hexafluorophosphate + Water and 1-Butyl-3-methylimidazolium Hexafluorophosphate + 1-Butanol by the Volumetric Method. *1st International Congress on Ionic Liquids (COIL), Book of Abstracts*, p. 269, Salzburg, Austria, 19-22 June 2005.
29. Eleftheriadis K., Ždímal V., Wagner Z., Vratolis S.: Performance Comparison of SMPS and LAS-X using Ammonium Sulphate and Sodium Chloride Aerosol. *European Aerosol Conference EAC 2005, Book of Abstracts*, p. 297, Ghent, Belgium, 28 August - 02 September 2005.

30. Fritz G., Tomšič M., Vlček L., Bergmann A., Nezbeda I., Jamnik A.: Structure of Simple Alcohols - Comparing Simulations with SAXS Measurements. 6th Liquid Matter Conference, Abstracts Book, p. 79, Utrecht, Netherlands, 02-06 July 2005.
31. Gonzales-Salgado D., Vlček L., Nezbeda I.: Excess Properties of Aqueous Mixtures of Methanol: Realistic and Primitive Models. Thermodynamics 2005, Book of Abstracts 158, p. 158, Sesimbra, Portugal, 06-08 April 2005.
32. Jirsák J., Nezbeda I.: Molecular Mechanisms Underlying the Thermodynamic Properties of Water. Thermodynamics 2005, Book of Abstracts, p. 104, Sesimbra, Portugal, 06-08 April 2005.
33. Krejčí J., Lísal M.: Simulation Study of Conformational Behavior of Model Linear Polymers in Vacuum. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.
34. Linek J., Morávková L., Wagner Z.: (P, V, T, x) Measurements of the Toluene + Propiophenone System at Temperatures from 298.15 K to 328.15 K and at Pressures Up to 40 MPa. Thermodynamics 2005, Book of Abstracts, p. 110, Sesimbra, Portugal, 06-08 April 2005.
35. Linek J., Morávková L., Wagner Z.: (P, V, T, x) Measurements of the Toluene + Propiophenone System at Temperatures from 298.15 K to 328.15 K and at Pressures Up to 40 MPa. 21st European Symposium on Applied Thermodynamics ESAT 2005, Proceedings, p. 60-62, Jurata, Poland, 01-05 June 2005.
36. Lísal M.: Monte Carlo Simulations in Unconventional Ensembles. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.
37. Lísal M., Nezbeda I.: Adiabatic Monte Carlo Simulation of Ammonia Synthesis Reaction. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 109, Tatranské Matliare, Slovakia, 23-27 May 2005.
38. Lísal M., Smith W.R.: Molecular Simulation of Electrolyte Chemical Potential for Concentrated Aqueous Electrolyte Solutions. Mainz Materials Simulations Days 2005 - MMSD 2005, Mainz, Germany, 08-10 June 2005.
39. Lísal M., Smith W.R.: Molecular Simulations of Open Electrolyte Solution Systems: The Expanded-Ensemble Osmotic Molecular Dynamics Method. 29th International Conference on Solution Chemistry, Book of Abstracts, p. 93, Portorož, Slovenia, 21-25 August 2005.
40. Lísal M., Smith W.R., Aim K., Bendová M.: Monte Carlo Simulations in Non-Traditional Ensembles. 6th Liquid Matter Conference, Abstracts Book, p. 64, Utrecht, Netherlands, 02-06 July 2005.
41. Morávková L., Aim K., Linek J.: Excess Molar Volumes of (Octane + 1-Chloropentane) at Temperatures between 298.15 K and 328.15 K and at Pressures Up to 40 MPa. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 176, Tatranské Matliare, Slovakia, 23-27 May 2005.
42. Moučka F., Nezbeda I.: A Quantitative Characterization of Structural Changes in the Hard-Disk Fluid Near Freezing/Melting Conditions. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.
43. Nezbeda I.: Molekulární simulace v chemickém inženýrství: Současný stav, problémy a perspektivy. (Czech) 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 54, Srní, Šumava, Czech Republic, 17-20 October 2005.
44. Nezbeda I.: Molecular Modeling of Fluids: From Realistic Hamiltonians to Simple Models and Their Applications. Thermodynamics 2005, Book of Abstracts, p. 67, Sesimbra, Portugal, 06-08 April 2005.
45. Nezbeda I., Gonzalez-Salgado D., Vlček L.: Excess Properties of Aqueous Mixtures of Methanol: Realistic and Primitive Models. 29th International Conference on Solution Chemistry, Book of Abstracts, p. 47, Portorož, Slovenia, 21-25 August 2005.
46. Nezbeda I., Moučka F.: Detection and Characterization of Structural Changes in the Hard-Disk Fluid Near Freezing/Melting Conditions. Mainz Materials Simulations Days 2005 - MMSD 2005, Book of Abstracts, Mainz, Germany, 08-10 June 2005.
47. Předota M.: Space-Dependent Diffusivity at Solid-Solid Interface. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.

48. Rouha M., Nezbeda I.: Calculation of Virial Coefficients of Primitive Models of Polar and Associating Fluids. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.
49. Siperstein F.R., Amat L., Lísal M.: Adsorption of Methane and Nitrogen in Titanosilicates. AIChE Annual Meeting, Cincinnati, OH, USA, 30 October - 04 November 2005.
50. Slovák J., Tanaka H.: The Stability Limit of Metastable Water Ices VII and XII from Computer Simulations: Comparison for Various Water Potentials. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.
51. Slovák J., Tanaka H.: Computer Simulation Study of Metastable Ice VII and Amorphous Phases Obtained by Its Melting. 6th Liquid Matter Conference, Abstracts Book, p. 268, Utrecht, Netherlands, 02-06 July 2005.
52. Škvor J., Nezbeda I.: Clustering and Percolation in Supercritical Fluids. European/Japanese Molecular Liquids Group Annual Meeting, Prague, Czech Republic, 04-08 September 2005.
53. Wichterle I., Aim K.: Vapor-Liquid Equilibrium Coupled with Chemical Reaction (Transesterification). 21st European Symposium on Applied Thermodynamics ESAT 2005, Proceedings, p. 68-69, Jurata, Poland, 01-05 June 2005.
54. Ždímal V., Schwarz J., Wagner Z., Dohányosová P., Smolík J.: The Dynamic of Atmospheric Aerosol Number Size Distributions at a Suburban Site in Prague. European Aerosol Conference EAC 2005, Book of Abstracts, p. 713, Ghent, Belgium, 28 August - 02 September 2005.
55. Předota M.: Dynamic and Structural Properties of Inhomogeneous Region at Solid-Liquid Interface. 29th International Conference on Solution Chemistry, Portorož, Slovenia, 21-25 August 2005.

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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
- Similarity approach to structure reactivity relationships
- Theoretical analysis of bonding changes and electron correlation in chemical reaction
- 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

Study of early ageing of hardened cement paste

(O. Šolcová, supported by GA CR, grant No. 106/03/0028)

Physical properties of the hardened cement paste exhibiting a great impact on practice are basically influenced by the nature of its porous structure. Origin of the pores is closely connected with the early stage of hydration process during which the calcium silicate hydrate (CSH) clusters are formed via nucleation and subsequent grows (solidification). This project focuses on the influence of the water to cement ratio both on the induction time of CSH nucleation and on the evolution of porosity in cement gels. The texture properties are correlated together with changes in electrical conductivity and the induction period of calcium silicate hydrates nucleation. [Refs. 4, 5, 42, 63, 65]

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 are applied together with newly obtained information on adsorbed film thickness. The obtained results are mutually correlated with pore structures established by high-resolution electron microscopy. [Refs. 1, 24, 38, 43, 46, 48, 50-52]

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 is applied. To decrease the number of fitted parameters, the axial dispersion parameter (Peclet number) is 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 are compared with characteristics from standard textural analyses. [Refs. 18, 33, 35, 60, 61, 64, 66]

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

(V. Hejtmánek, supported by GA ASCR, 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. 24, 43]

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 results obtained were presented in a number of contributions in scientific journals and international symposia. [Refs. 9, 18, 24, 35, 43, 50-55, 60, 61]

Molybdenum sulfide catalysts promoted by dispersed Ru and Pt sulfides

(Z. Vít, supported by ICPF AS CR)

The effect of Ru and Pt added to a Mo/Al₂O₃ catalyst on activity in hydrosulfurization of thiophene and hydrogenation of cyclohexene was studied. The effect of Ru was greater than that of Pt. The strong synergetic effect of Ru in hydrogenation was accompanied by

increase of the apparent activation energy and explained by participation of the Ru-Mo-S sites [Ref. 19]. The activity and selectivity of alumina and silica-alumina supported Mo catalysts promoted by Pt was compared in hydrodesulfurization/hydrodenitrogenation of thiophene and pyridine. The strong effect of support acidity was observed mainly in the C-N bond cleavage of piperidine. It led to overall higher hydrodenitrogenation activity and substantially improved hydrodenitrogenation/hydrodesulfurization selectivity [Ref. 67].

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. [Refs. 16, 17, 31, 32, 62]

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 catalyst having various molar ratios of Co:Mg:Mn:Al. The Co₄MnAl catalyst is the most active as it shows optimum ratio of compounds reducible in the temperature range 350-450 °C in which catalytic reaction proceeds. [Refs. 9, 27, 29, 49, 56]

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. [Refs. 3, 8, 26, 37, 41, 45, 53-55, 57, 59]

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)

The monolayer MoO₃/Al₂O₃ catalysts were prepared by the reaction of alumina with the slurry MoO₃/water using fifteen different aluminas with surface area 11-279 m² g⁻¹. The amount of deposited MoO₃ and activity in hydrodesulfurization of thiophene were proportional to alumina surface area. Temperature programmed reduction showed that the character of the deposited monolayer was the same for all catalysts [Ref. 6]. Catalyst MoO₃/γ-Al₂O₃ was prepared by the reaction of α-boehmite with molybdic acid in slurry MoO₃/H₂O followed by calcination. The deposited MoO₃ functioned simultaneously as active phase and thermal stabilizer, which inhibited sintering of Al₂O₃ phase during calcination [Refs. 7, 48].

Role of electron pairing in chemical bonds

(R. Ponc, 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. [Refs. 13-15, 23, 30, 34], to the description of bonding in infinite periodical structures (solids) [Ref. 10], and to the quantitative characterization of the extended cyclic delocalization in aromatic hydrocarbons [Refs. 2, 11, 12, 20, 21, 39, 40].

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. [Refs. 22, 58]

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 Pais Vasco, Bilbao, Spain: Analysis of the pair density matrix

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

Teaching

R. Ponec: CU, course "Reaction mechanisms in organic chemistry"

P. Schneider: ICT, postgraduate course "Texture of porous solids"

Publications

Original papers

1. Brabec L., Novák P., Šolcová O., Kočířík M.: Polycrystalline Silicalite-1 Layers: Texture and Kinetics of Growth. *Micropor. Mesopor. Mat.* 78(1), 29-36 (2005).
2. Bultinck P., Ponec R., Van Damme S.: Multicenter Bond Indices as a New Measure of Aromaticity in Polycyclic Aromatic Hydrocarbons. *J. Phys. Org. Chem.* 18(8), 706-718 (2005).
3. Dobrosz I., JirátoVá K., Pitchon V., Rynkowski J.M.: Effect of the Preparation of Supported Gold Particles on the Catalytic Activity in CO Oxidation Reaction. *J. Mol. Catal.* 234(1-2), 187-197 (2005).
4. Dříněk V., Vacek K., Pola J., Yuzhakov G., Šolcová O., Naumov S.: Characterization of Deposits Produced by TEA CO₂ Pulsed Laser Ablation of Silicon Mono- and Dioxide. *J. Non-Cryst. Solids* 351(2), 116-123 (2005).
5. Hartman M., Trnka O., Šolcová O.: Thermal Decomposition of Aluminium Chloride Hexahydrate. *Ind. Eng. Chem. Res.* 44(17), 6591-6598 (2005).
6. Kaluža L., Vít Z., Zdražil M.: Preparation and Properties of Filled Monolayer of MoO₃ Deposited on Al₂O₃ Supports by Solvent-Assisted Spreading. *Appl. Catal. A* 282(1-2), 247-253 (2005).
7. Kaluža L., Zdražil M.: Preparation of MoO₃/gamma-Al₂O₃ Catalyst by the Reaction of alpha-Boehmite with MoO₃/H₂O Slurry - Dual Role of MoO₃ as Active Phase and Texture Stabilizer during Calcination. *React. Kinet. Catal. Lett.* 85(2), 391-398 (2005).
8. Kovanda F., Grygar T., Dorničák V., Rojka T., Bezdička P., JirátoVá K.: Thermal Behaviour of Cu-Mg-Mn and Ni-Mg-Mn Layered Double Hydroxides and Characterization of Formed Oxides. *Appl. Clay Sci.* 28(1-4), 121-136 (2005).
9. Obalová L., JirátoVá K., Kovanda F., Pacultová K., Lacný Z., Mikulová Z.: Catalytic Decomposition of Nitrous Oxide over Catalysts Prepared from Co/Mg-Mn/Al Hydrotalcite-like Compounds. *Appl. Catal. B* 60(3-4), 289-297 (2005).
10. Ponec R.: Chemical Bonding in Solids. On the Generalization of the Concept of Bond Order and Valence for Infinite Periodical Structures. *Theor. Chem. Acc.* 114(1-3), 208-212 (2005).
11. Ponec R., Bultinck P., Gallegos A.: Multicenter Bond Indices as a New Means for the Quantitative Characterization of Homoaromaticity. *J. Phys. Chem. A* 109(29), 6606-6609 (2005).
12. Ponec R., Bultinck P., Van Damme S., Carbó-Dorca R., Tantillo D.J.: Geometric and Electronic Similarities between Transition Structures for Electrocyclizations and Sigmatropic Hydrogen Shifts. *Theor. Chem. Acc.* 113(4), 205-211 (2005).
13. Ponec R., Cooper D.: Anatomy of Bond Formation. Bond Length Dependence of the Extent of Electron Sharing in Chemical Bonds. *J. Mol. Struct.-Theochem* 727(1-3), 133-138 (2005).
14. Ponec R., Chaves J.: Electron Pairing and Chemical Bonds. Electron Fluctuation and Pair Localization in ELF Domains. *J. Comput. Chem.* 26(12), 1205-1213 (2005).
15. Ponec R., Yuzhakov G., Sundberg M.R.: Chemical Structures from the Analysis of Domain - Averaged Fermi Holes. Nature of the Mn-Mn Bonding in Bis(Pentacarbonyl-manganese). *J. Comput. Chem.* 26(5), 447-454 (2005).
16. Spojakina A.A., Králeva E., JirátoVá K., Petrov L.: TiO₂-Supported Iron-Molybdenum Hydrodesulfurization Catalysts. *Appl. Catal., A* 288(1-2), 10-17 (2005).

17. Spojakina A.A., Palcheva R., Jiráťová K., Tyuliev G., Petrov L.: Synergism between Ni and W in the NiW/gama-Al₂O₃ Hydrotreating Catalysts. *Catal. Lett.* 104(1-2), 45-52 (2005).
18. Šolcová O., Soukup K., Schneider P.: Axial Dispersion in Single Pellet-String Columns Packed with Unusually Shaped Porous Pellets. *Chem. Eng. J.* 110(1-3), 11-18 (2005).
19. Vít Z., Gulková D., Kaluža L., Zdražil M.: Synergetic Effects of Pt and Ru Added to Mo/Al₂O₃ Sulfide Catalyst in Simultaneous Hydrodesulfurization of Thiophene and Hydrogenation of Cyclohexene. *J. Catal.* 232(2), 447-455 (2005).
20. Bultinck P., Ponec R., Carbó-Dorca R.: Aromaticity in Linear Polyacenes Generalize Population Analysis and Molecular Quantum Similarity Approach. *J. Phys. Chem.*, submitted.
21. Bultinck P., Ponec R., Gallegos A., Fias S., Van Damme S., Carbó-Dorca R.: Generalized Polansky Index as a New Means for the Quantitative Characterization of Aromaticity in Polycyclic Aromatic Hydrocarbons. *Croat. Chem. Acta*, submitted.
22. Girónes X., Ponec R.: Molecular Quantum Similarity Measures from Fermi Hole Densities. Modelling of Hammett Sigma Constants. *J. Chem. Inf. Modell.*, in press.
23. Gulková D., Kaluža L., Vít Z., Zdražil M.: Preparation of MoO₃/MgO Catalysts with Eggshell and Uniform Mo Distribution by Methanol Assisted Spreading: Effect of MoO₃ Dispersion on Rate of Spreading. *Catal. Commun.*, in press.
24. Hejtmánek V., Schneider P., Soukup K., Šolcová O.: Comparison of Transport Characteristics and Textural Properties of Porous Material; the Role of Pore Sizes and Their Distributions. *Stud. Surf. Sci. Catal.*, in press.
25. Kaluža L., Gulková D., Zdražil M.: Preparation of Eggshell MoO₃/Al₂O₃ Catalysts by Solvent Assisted Spreading of MoO₃ over Al₂O₃ Extrudates: Effect of MoO₃ Particle Size and Temperature on Rate of Spreading. *Materials Science: An Indian Journal*, in press.
26. Kašťánek F., Maléterová Y., Kašťánek P., Rott J., Jiříčný V., Jiráťová K.: Complex Treatment of Soils, Waste Water and Groundwater Contaminated by Halogenated Organic Compounds. *Desalination*, in press.
27. Kovanda F., Rojka T., Dobešová J., Machovic V., Bezdička P., Obalová L., Jiráťová K., Grygar T.: Mixed Oxides Obtained from Co and Mn Containing Layered Double Hydroxides: Preparation, Characterization, and Catalytic Properties. *J. Solid State Chem.*, in press.
28. Klusoň P., Lusková H., Cajthaml T., Šolcová O.: Non Thermal Preparation of Photoactive Titanium (IV) Oxide Thin Layers. *Thin Solid Films*, in press.
29. Obalová L., Jiráťová K., Kovanda F., Valášková M., Balabánová J., Pacultová K.: Characterization of Calcined Ni-(Mg)-MIII (MIII = Al or Mn) Layered Double Hydroxides and Their Activity in N₂O Decomposition. *J. Mol. Catal. A-Chem.*, in press.
30. Ponec R., Bultinck P., Gupta P., Tantillo D.J.: Multicenter Bonding in Carbocations with Tetracoordinated Proton. *J. Phys. Chem.*, submitted.
31. Spojakina A.A., Kraleva E.U., Jiráťová K., Kociánová J., Petrov L.A.: FePMo₁₂O₄₀ Heteropolycompounds in Preparation of Hydrodesulfurization Catalysts. *Bulgar. Chem. Commun.*, submitted.
32. Spojakina A.A., Palcheva R., Kostova N.G., Jiráťová K., Tyuliev G., Petrov L.A.: Mutual Effect of Ni and W on Properties of NiW/Al₂O₃ Catalysts for Hydrodesulfurization. *Appl. Catal., A*, submitted.
33. Starý T., Šolcová O., Schneider P., Marek M.: Effective Diffusivities and Pore-Transport Characteristics of Washcoated Ceramic Monolith for Automotive Catalytic Converter. *Appl. Catal., B*, submitted.

34. Sundberg M., Ponec R.: The Nature of M-O Bond in MOX₄ Compounds (M=Os,Ru; X=F,Cl,Br,I). *Inorg. Chim. Acta*, in press.
35. Šolcová O., Soukup K., Schneider P.: Diffusion Coefficients and Other Transport Characteristics of Peculiarly Shaped Porous Materials in the Single-Pellet-String Column. *Micropor. Mesopor. Mat.*, in press.

Chapters in books

36. Gironés X., Ponec R.: Molecular Quantum Similarity Measures from Fermi Hole Densities. Modelling of Hammett Sigma Constants. In: *Molecular Similarity. Concepts and Applications*. (Carbó-Dorca, R., Ed.), Nova Publishers, New York, in press.
37. Kovanda F., Jirátovej K., Kalousková R.: Synthetic Hydrotalcite-like Compounds. In: *Advances in Chemistry Research.*, Nova Science Publishers, in press.
38. Šolcová O., Schneider P.: Experimental Determination of Transport Parameters. In: *Gas Transport in Porous Media*. (Clifford, K. Ho - Webb, S.W. - Wilson, J., Ed.), Howell, K., in press.

Conferences

39. Bultinck P., Carbó-Dorca R., Ponec R.: Generalized Population Analysis and Molecular Quantum Similarity for Molecular Aromaticity. ICCMSE 2005 International Conference on Computational Methods in Sciences and Engineering, Final Program, p. 1-3, Loutraki, Corinth, Greece, 21-26 October 2005.
40. Bultinck P., Gallegos A., Van Damme S., Ponec R., Carbó-Dorca R.: A Molecular Quantum Similarity Approach to Aromaticity. MATH/CHEM/COMP2005 Dubrovnik International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Program & Book of Abstracts, p. 9, Dubrovnik, Croatia, 20-25 June 2005.
41. Čuba P., Kovanda F., Hilaire L., Jirátovej K.: Properties and Oxidation Activity of the Calcined Mn-Containing Hydrotalcite-like Compounds. 4th International Conference on Environmental Catalysis, Programme/Book of Abstracts, p. 231, Heidelberg, Germany, 05-08 June 2005.
42. Dřínek V., Fajgar R., Schneider P., Šnajdaufová H., Šolcová O.: Textural Properties of Silicon Materials Produced by Laser Action. 7th International Symposium on the Characterisation of Porous Solids COPS VII, Abstracts, p. 50, Aix-en-Provence, France, 25-28 May 2005.
43. Hejtmánek V., Schneider P., Soukup K., Šolcová O.: Comparison of Transport Characteristics and Textural Properties of Porous Material; the Role of Pore Size and Their Distributions. 7th International Symposium on the Characterisation of Porous Solids COPS VII, Abstracts, p. 58, Aix-en-Provence, France, 25-28 May 2005.
44. Jirátovej K., Markvart M.: Use of Waste Salts Remaining in the Underground after Chemical Mining of Uranium Ore. 4th International Conference on Environmental Catalysis, Programme/Book of Abstracts, p. 296, Heidelberg, Germany, 05-08 June 2005.
45. Jirátovej K., Rymeš J., Čuba P., Balabánová J., Bohmová V.: Pt/TiO₂ Catalyst in Total Oxidation of VOC. Joint with 1st Czech-Italian Workshop on Catalysis and Zeolites, Proceedings, p. 59-62, Camigliatello Silano, Italy, 26-30 June 2005.
46. Jirglová H., Zikánová A., Kočičík M., Šolcová O., Kortunov P., Vasenkov S., Kaerger J., Krystl V., Bernauer B., Drescher B.: Transport Related Structure Characteristics of FCC Catalysts from Sorption, Porosimetric and PFG NMR Measurements. 3rd International

- FEZA Conference, Book of Abstracts, p. 1-2, Praha, Czech Republic, 23-26 August 2005.
47. Kaluža L., Gulková D., Zdražil M.: Preparation of Eggshell MoO₃/Al₂O₃ Catalyst by Solvent-Assisted Spreading: Effect of MoO₃ Origin and Activation. 7th European Congress on Catalysis EUROPACAT-VII, Book of Abstracts, p. 30 (P1-08), Sofia, Bulgaria, 28 August - 01 September 2005.
 48. Kaluža L., Zdražil M.: Preparation of MoO₃/gamma-Al₂O₃ Catalyst by the Reaction of alpha-Boehmite with MoO₃/H₂O Slurry - Dual Role of MoO₃ as Active Phase and Texture Stabilizer during Calcination. XXXVII Symposium on Catalysis, Book of Abstract, p. 43-44, Praha, Czech Republic, 07-08 November 2005.
 49. Kovanda F., Rojka T., Jirátovej K., Obalová L., Grygar T.: Směsné oxidy připravené tepelným rozkladem Co-Mn-Al hydrotalcitů a jejich katalytické vlastnosti. (Czech) Mixed Oxides Prepared from Co-Mn-Al Hydrotalcite-like Compounds by Calcination and Their Catalytic Properties. 57. zjazd chemických společností, ChemZi 1/1 2005, p. 81 (2P12), Tatranské Matliare, Slovakia, 04-08 September 2005.
 50. Matějová L., Klusoň P., Lusková H., Schneider P., Šolcová O.: Nanoporous Materials with Narrow Monodisperse Pore-Size Distributions: Corning Controlled Porous Glasses and TiO₂. International Course New Trends in Catalysis, Proceedings, p. 201-202, Brussels, Belgium, 11-13 October 2005.
 51. Matějová L., Šnajdaufová H., Šolcová O., Schneider P.: Adsorption Measurements of Monodisperse Corning Porous Glasses; Standard Isotherm for t- and ú- Plots. 7th International Symposium on the Characterisation of Porous Solids COPS VII, Abstracts, p. 81, Aix-en-Provence, France, 25-28 May 2005.
 52. Matějová L., Šolcová O., Klusoň P., Lusková H.: Řízená příprava nanoporézního TiO₂ s úzkou distribucí pórů pro adsorpční měření. (Czech) Preparation of Nanoporous TiO₂ with Narrow Pore-Size Distribution. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 135, Srní, Šumava, Czech Republic, 17-20 October 2005.
 53. Mikulová Z., Balabánová J., Jirátovej K., Kovanda F.: Properties and Activity of Calcined Co(Mg)Al(Mn) Hydrotalcite-like Precursors in Total Oxidation of VOC. International Course New Trends in Catalysis, Proceedings, p. 199-200, Brussels, Belgium, 11-13 October 2005.
 54. Mikulová Z., Balabánová J., Kovanda F., Bastl Z., Jirátovej K.: Calcined Co(Mg)Al(Mn) Hydrotalcite-like Precursors in Total Oxidation of VOC. XXXVII Symposium on Catalysis, Book of Abstracts, p. 31-32, Prague, Czech Republic, 07-08 November 2005.
 55. Mikulová Z., Balabánová J., Kovanda F., Jirátovej K.: Properties and Activity of Calcined Co(Mg)Al(Mn) Hydrotalcite-like Precursors in Total Oxidation of VOC. 7th European Congress on Catalysis EuropaCat-VII, Book of Abstracts, p. 291 (P9-50), Sofia, Bulgaria, 28 August - 01 September 2005.
 56. Pacultová K., Obalová L., Balabánová J., Jirátovej K., Valášková M.: Catalytic Decomposition of N₂O over Co-Mn-Al Catalysts Prepared from Hydrotalcite-like Precursors with Different Mn/Al Ratio. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 107, Tatranské Matliare, Slovakia, 23-27 May 2005.
 57. Patera J., Krupka J., Jirátovej K.: Příprava Pd/Al₂O₃ katalyzátorů mikroemulzní technikou. (Czech) Preparation of Pd/Al₂O₃ Catalysts by Microemulsion Technique. 57. zjazd chemických společností, ChemZi 1/1 2005, p. 120 (6P17), Tatranské Matliare, Slovakia, 04-08 September 2005.
 58. Ponec R.: Molecular Basis of LFER. Simple Model for the Estimation of Brønsted Exponent in Acidobasis Catalysis. MATH/CHEM/COMP 2005 Dubrovnik International

- Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences, Program & Book of Abstracts, p. 60, Dubrovnik, Croatia, 20-25 June 2005.
59. Rymeš J., JirátoVá K., Hilaire L.: Total Oxidation of Ethanol over Supported Pt Catalysts. 4th International Conference on Environmental Catalysis, Programme/Book of Abstracts, p. 232, Heidelberg, Germany, 05-08 June 2005.
 60. Schneider P., Součková H., Soukup K., Šolcová O.: Transport Parameters and Diffusion Coefficients of Catalysts with Complex Shapes from Chromatographic Measurements. 7th International Symposium on the Characterisation of Porous Solids COPS VII, Abstracts, p. 116, Aix-en-Provence, France, 25-28 May 2005.
 61. Soukup K., Šolcová O., Schneider P.: Transportní parametry a texturní vlastnosti porézních látek. (Czech) Transport Parameters and Textural Properties of Porous Solids. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 131, Srní, Šumava, Czech Republic, 17-20 October 2005.
 62. Spojakina A.A., Kraleva E., JirátoVá K., Petrov L.: Support Effect of the Formation of Catalytic Sites Precursors Active in Thiophene Hydrodesulfurization. 4th International Conference on Environmental Catalysis, Programme/Book of Abstracts, p. 269, Heidelberg, Germany, 05-08 June 2005.
 63. Starý T., Šolcová O., Schneider P., Marek M.: Effective Diffusivities and Pore-Transport Characteristics of Washcoated Monolith by Chromatographic Technique. 2nd International Conference on Structured Catalysts and Reactors, Book of Abstracts, p. 1, Delft, Netherlands, 16-19 October 2005.
 64. Starý T., Šolcová O., Schneider P., Marek M., Schejbal M.: Effective Diffusivities and Pore-Transport Characteristics of Washcoated Monolith for Automotive Catalytic Converter. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 125, Srní, Šumava, Czech Republic, 17-20 October 2005.
 65. Starý T., Šolcová O., Schneider P., Marek M.: Effective Diffusivities and Pore-Transport Characteristics of Washcoated Ceramic Monolith for Automotive Catalytic Converter. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 215, Tatranské Matliare, Slovakia, 23-27 May 2005.
 66. Šolcová O., Schneider P.: Distribution of Through-Pore Sizes from Liquid Expulsion Termoporometry. 1st International Workshop Macro/Mesopore Analysis: Mercury Porosimetry and Alternative Liquid Penetration Techniques, Book of Abstracts, p. 17, Aix-en-Provence, France, 30-31 May 2005.
 67. Vít Z., Gulková D.: Effect of Support Acidity on Activity and Selectivity of Pt-Mo Catalysts in HDS/HDN Reaction of Thiophene and Pyridine. XXXVII Symposium on Catalysis, Book of Abstracts, p. 40, Prague, Czech Republic, 07-08 November 2005.

Department of Multiphase Reactors

Head: J. Drahoš
Deputy: J. Tihon
Research staff: M. Fialová, M. Fugasová, J. Havlica, 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, P. Stanovský, M. Šimčík

Fields of research

- Hydrodynamics and transport phenomena in different types of gas-liquid, liquid-solid or gas-liquid-solid reactors
- 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. 2, 3, 13, 17-20, 47-50, 52-58, 61, 62, 65, 73]

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

(O. Wein, joint project with Institute of Hydrodynamics ASCR Prague, 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. 11, 12, 71]

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. 8, 35-37, 46, 59, 60]

Hydrodynamic interactions of bubbles and particles in flotation process

(M. Růžička, joint project with ICT Prague, 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 interactions between bubbles and solids. [Refs. 21-25, 30-36, 45]

Collision dynamics of bubbles and solid particles in liquids

(J Havlica, supported by GA CR, grant No. GA104/05/P554)

The suggested 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. 30-34]

Study of the bubble growth during boiling

(J Vejražka, supported by GA CR, grant No. GA104/05/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. 49, 69, 70]

Reaction and transport phenomena in complex homogeneous and heterogeneous systems

(J. Drahoš, joint project with ICT, Prague, 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. 17-25, 29, 49, 50, 52-58, 61, 62]

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 EU 5th RTD 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. 2, 5, 13, 20-22, 31]. 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, Refs. 22, 23] 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 Diffusion and Separation Processes, Refs. 11, 23, 24, 33, 62].

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" will be organized in the frame of the international congress "CHISA2006". [Refs. 38-43]

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 (4 months)
M. Pantzali, Aristotle University, Thessaloniki, Greece (1 month)
F. Huchet, University of Nantes, France
J. Comiti, University of Nantes, France
T. Bonometti, Institute of Fluid Mechanics, Toulouse, France
A. Tomiyama, Kobe University, Japan
R. Mudde, Delft TU, Delft, The Netherlands
G. Trygvasson, Worcester Polytechnic Institute, Worcester, USA
I. Zun, University of Ljubljana, Slovenia
G.P. Celata, ENEA, Italy
J. Magnaudet, Institute of Fluid Mechanics, Toulouse, France
E.J. Hinch, University of Cambridge, UK

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"

Publications

Original papers

1. Jirout T., Moravec J., Rieger F.E., Sinevič V., Špidla M., Sobolík V., Tihon J.: Electrochemical Measurement of Impeller Speed for Off-Bottom Suspension. *Inz. Chem. Procesowa* 26(3), 485-497 (2005).
2. Mena P.C., Růžička M., Rocha F.A., Teixeira J.A., Drahoš J.: Effect of Solids on Homogeneous-Heterogeneous Flow Regime Transition in Bubble Columns. *Chem. Eng. Sci.* 60(22), 6013-6026 (2005).
3. Punčochář M., Drahoš J.: Origin of Pressure Fluctuations in Fluidized Beds. *Chem. Eng. Sci.* 60(5), 1193-1197 (2005).
4. Růžička M.: Vertical Stability of Uniform Bubble Chain. *Int. J. Multiphase Flow* 31(10-11), 1063-1096 (2005).
5. Vejražka J., Tihon J., Marty P., Sobolík V.: Effect of an External Excitation on the Flow Structure in a Circular Impinging Jet. *Phys. Fluids* 17(10), 105102 (2005).
6. Wein O.: Viscometric Flow under Apparent Wall Slip in Parallel-Plate Geometry. *J. Non-Newtonian Fluid Mech.* 126(2-3), 105-114 (2005).
7. Fujasová M., Vejražka J., Moucha T., Linek V.: Spatial Distribution of Energy Dissipation Intensity in Gas-Liquid Dispersion Agitated by Various Impellers. *Chem. Eng. Sci.*, submitted.
8. Huchet F., Comiti J., Tihon J., Montillet A., Legentilhomme P.: Electrodiffusion Diagnostics of the Flow and Mass Transfer inside a Network of Crossing Minichannels. *J. Appl. Electrochem.*, submitted.
9. Tihon J., Serifi K., Argyriadi K., Bontozoglou V.: Solitary Waves on Inclined Films: Their Characteristics and the Effect on Wall Shear Stress. *Exp. Fluids*, submitted.
10. Vejražka J., Marty P.: An Alternative Technique for Interpretation of the Temperature Measurements using Thermochromic Liquid Crystals. *Heat Transfer Eng.*, in press.
11. Wein O., Večeř M., Tovčigrečko V.V.: AWS Rotational Viscometry of Polysaccharide Solutions Using a Novel KK Sensor. *J. Non-Newtonian Fluid Mech.*, submitted.
12. Wein O., Tovčigrečko V., Sobolík V.: Transient Convective Diffusion to a Circular Sink at Finite Peclet Number. *Int. J. Heat Mass Transfer*, submitted.

Chapters in books

13. Drahoš J., Růžička M.: Time Series Analysis in Characterization of Process Data. In: 8th Conference of Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction Pres'05. (Klemeš, J., Ed.), pp. 607-613, AIDIC Servizi S.r.l., Milano 2005.

Patents

14. Hájek M., Drahoš J., Volf V., Vozáb J.: Method and Apparatus for Heat Treatment of Glass Material and Natural Materials Specifically of Volcanic Origin. Pat. No. 6,938,441 B1/10/018,119. Applied: 00.06.12, Granted: 05.09.06.
15. Hájek M., Drahoš J., Volf V., Vozáb J.: Sposob a zariadenie na tepelné zpracovanie 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. 284 512/1690-2001. Applied: 00.06.12, Granted: 05.05.05.

Conferences

16. Andertová J., Tláškal R., Havrda J., Večeř M.: Rheological Behavior of Suspensions for Preparation of Functionally Graded Alumina Ceramic Materials. 2nd Annual European Rheology Conference AERC 2005, Abstracts, p. 95, Grenoble, France, 21-23 April 2005.
17. Bunganič R., Růžička M., Drahoš J.: Vybrané aspekty tvorby bublín na jednom otvore. (Slov) Chosen Aspects of Bubble Formation at One Orifice. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 232, Srní, Šumava, Czech Republic, 17-20 October 2005.
18. Bunganič R., Růžička M., Drahoš J.: Režimy tvorby bublín na dvoch otvoroch. (Slov). Regimes of Bubble Formation at Two Orifices. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 59, Srní, Šumava, Czech Republic, 17-20 October 2005.
19. Bunganič R., Růžička M., Drahoš J.: Experimentálne štúdium tvorby bublín: akustika a ccd kamera. (Slov). Experimental Study of Bubble Formation: Acoustics and CDD Camera. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 222, Srní, Šumava, Czech Republic, 17-20 October 2005.
20. Bunganič R., Růžička M., Drahoš J.: Multiple Bubble Formation: Experiments and Modelling. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 1.2.3., Strasbourg, France, 21-24 August 2005.
21. Bunganič R., Růžička M., Drahoš J.: Some Aspects of Single Bubble Formation. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.4., Strasbourg, France, 21-24 August 2005.
22. Bunganič R., Růžička M., Drahoš J.: The Experimental Study of Bubble Formation: Acoustics and CCD Camera. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.5., Strasbourg, France, 21-24 August 2005.
23. Bunganič R., Růžička M., Drahoš J.: The Simultaneous Bubble Formation at Two Orifices. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 38, Tatranské Matliare, Slovakia, 23-27 May 2005.
24. Bunganič R., Růžička M., Drahoš J.: A Case Study of Single Bubble Formation. 43rd European Two-Phase Flow Group Meeting 2005, Program & List of Participants, Prague, Czech Republic, 11-13 May 2005.
25. Bunganič R., Růžička M., Drahoš J.: The Influence of Control Parameters on Bubble Formation. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 236, Tatranské Matliare, Slovakia, 23-27 May 2005.
26. Fialová M., Blažej M., Drahoš J., Linek V., Růžička M.: Using of Dynamic Pressure Step Method for Volumetric Mass Transfer Coefficient Measurement in Bubble Column. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 239, Tatranské Matliare, Slovakia, 23-27 May 2005.
27. Fialová M., Drahoš J.: Regime Transition in Bubble Columns: Comparison of Experiments with Predictions from Literature. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 278, Tatranské Matliare, Slovakia, 23-27 May 2005.
28. Fijasová M., Vejražka J., Moucha T., Linek V.: Spatial Distribution of Energy Dissipation Intensity in Gas-Liquid Dispersion Agitated by Various Impellers. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 41, Tatranské Matliare, Slovakia, 23-27 May 2005.
29. Gogová Z., Čamaj V., Markoš J.: Návrh a optimalizácia reaktora na výrobu propylénchlórhydrínu. (Slov). Design and Optimization of the Reactor for Propylene Chlorohydrin Production. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 198, Srní, Šumava, Czech Republic, 17-20 October 2005.
30. Havlica J., Bunganič R., Šimčík M., Růžička M., Drahoš J.: Bubble Formation and Detachment from Submerged Nozzles. 43rd European Two-Phase Flow Group Meeting 2005, Program & List of Participants, Prague, Czech Republic, 11-13 May 2005.

31. Havlica J., Bunganič R., Šimčík P., Růžička M., Drahoš J.: Bubble Formation on Submerged Needles and Orifices: CFD and Fast Camera. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.10., Strasbourg, France, 21-24 August 2005.
32. Havlica J., Bunganič R., Večeř M., Růžička M., Drahoš J.: Bubble Formation: Experiments and CFD Simulations. 11th Workshop on Two-Phase Flow Predictions, Book of Abstracts, p. 1, Merseburg, Germany, 05-08 April 2005.
33. Havlica J., Šimčík M., Bunganič R., Růžička M., Drahoš J.: Bubble Formation: Experiments and CFD Simulations. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 45, Tatranské Matliare, Slovakia, 23-27 May 2005.
34. Havlica J., Šimčík M., Bunganič R., Růžička M., Drahoš J.: Generování bublin: experiment a CFD simulace. (Czech) Generation of Bubbles: Experiments and CFD Simulations. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 55, Srní, Šumava, Czech Republic, 17-20 October 2005.
35. Havlica J., Tihon J.: Numerické simulace proudění v kanále za náhlým rozšířením. (Czech) Numerical Simulations of the Backward-Facing Step Flow. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 227, Srní, Šumava, Czech Republic, 17-20 October 2005.
36. Havlica J., Tihon J.: Numerical Simulations of the Backward-Facing Step Flow. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 172, Tatranské Matliare, Slovakia, 23-27 May 2005.
37. Huchet F., Comiti J., Legentilhomme P., Montillet A., Tihon J.: Etude hydrodynamique d'un réseau de mini-canaux croisés. (Fr) Study of Hydrodynamics inside a Network of Crossing Minichannels. 10 Congrès de la Société Française de Génie des Procédés, Récent Progrès an Génie des Procédés, p. R-16, Toulouse, France, 20-22 September 2005.
38. Křišťál J., Havlica J., Jiříčný V.: Porovnání 2D a 3D simulací proudění v mikroreaktoru. (Czech) 2D and 3D CFD Flow Simulations in Micro Reactor-Comparison. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 230, Srní, Šumava, Czech Republic, 17-20 October 2005.
39. Křišťál J., Havlica J., Jiříčný V.: Simulace proudění v reaktoru s úzkou štěrbinou. (Czech) CFD Flow Simulation in Narrow Channel. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 46, Srní, Šumava, Czech Republic, 17-20 October 2005.
40. Křišťál J., Havlica J., Jiříčný V.: Experimental Study of Bubbly Flow in a Thin-Gap Microreactor. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.11., Strasbourg, France, 21-24 August 2005.
41. Křišťál J., Havlica J., Jiříčný V.: Numerical Simulation of Single Bubble Rise in a Thin-Gap Microreactor. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.12., Strasbourg, France, 21-24 August 2005.
42. Křišťál J., Havlica J., Jiříčný V.: CFD Simulation of Gas-Liquid Flow in Thin-Gap Channel. 11th Workshop on Two-Phase Flow Predictions, Book of Abstracts, p. 1, Merseburg, Germany, 05-08 April 2005.
43. Křišťál J., Havlica J., Jiříčný V.: CFD Simulation of Gas-Liquid Flow in Narrow Channel. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 40, Tatranské Matliare, Slovakia, 23-27 May 2005.
44. Macháčová K., Raška P., Wichterle K., Večeř M., Růžička M.: Periodicita pohybu kolébajících se elipsoidálních bublin. (Czech) Movement Periodicity of Wobbling Ellipsoidal Bubbles. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 229, Srní, Šumava, Czech Republic, 17-20 October 2005.
45. Mena P.C., Růžička M., Rocha F.A., Teixeira J.A., Drahoš J.: Effects of Solids on Homogeneous-Heterogeneous Flow Regime Transition in Bubble Columns. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 1.1.14., Strasbourg, France, 21-24 August 2005.
46. Mouza A.A., Pantzali M.N., Paras S.V., Tihon J.: Experimental and Numerical Study of Backward-Facing Step Flow. 5th Hellenic Chemical Engineering Conference, Book of Abstracts, p. 1-4, Thessaloniki, Greece, 26-28 May 2005.

47. Růžička M., Drahoš J.: Scale-Up of Discrete Bubble Equations. Euromech Colloquium 465 on Hydrodynamics of Bubbly Flows, Book of Abstracts, p. 12, Lorentz Center, Leiden, Netherlands, 06-08 June 2005.
48. Růžička M., Večeř M., Drahoš J., Plzáková M., Wichterle K.: Multiscale Nature of Gas-Liquid Systems. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 235, Tatranské Matliare, Slovakia, 23-27 May 2005.
49. Stanovský P., Havlica J., Vejražka J., Růžička M., Drahoš J., Wichterle K.: Controlled Production of Bubbles of Desired Parameters. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 277, Tatranské Matliare, Slovakia, 23-27 May 2005.
50. Stanovský P., Růžička M., Drahoš J., Wichterle K.: Experiments on Spontaneous Bubble Production at $Re \sim 10^2$. 43rd European Two-Phase Flow Group Meeting 2005, Program & List of Participants, Prague, Czech Republic, 11-13 May 2005.
51. Staykov P., Fialová M., Vlaev S.D.: Computational Flow Modeling of a Bubble Column Reactor with Emphasis on Gas Hold-up Distribution. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 240, Tatranské Matliare, Slovakia, 23-27 May 2005.
52. Šimčík M., Havlica J., Růžička M., Drahoš J.: CFD of Gas-Liquid Flow in Bubble Column. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 237, Tatranské Matliare, Slovakia, 23-27 May 2005.
53. Šimčík M., Havlica J., Růžička M., Drahoš J.: CFD of Rising Bubbles. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 39, Tatranské Matliare, Slovakia, 23-27 May 2005.
54. Šimčík M., Havlica J., Růžička M., Drahoš J.: VOF Simulation of Rising Bubbles. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 56, Srní, Šumava, Czech Republic, 17-20 October 2005.
55. Šimčík M., Havlica J., Stanovský P., Růžička M., Drahoš J.: 2D Bubble Path Oscillations: Simulation vs. Experiment. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.9., Strasbourg, France, 21-24 August 2005.
56. Šimčík M., Stanovský P., Růžička M., Drahoš J.: A Case Study of 2D Bubble Rise. 43rd European Two-Phase Flow Group Meeting 2005, Program & List of Participants, Prague, Czech Republic, 11-13 May 2005.
57. Šimčík M., Stanovský P., Růžička M., Drahoš J.: Simulation of Motion of 2D Bubbles with Fluent. 11th Workshop on Two-Phase Flow Predictions, Book of Abstracts, p. 1, Merseburg, Germany, 05-08 April 2005.
58. Šimčík M., Večeř M., Havlica J., Růžička M., Drahoš J.: CFD Simulations of Rectangular Bubble Column. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 221, Srní, Šumava, Czech Republic, 17-20 October 2005.
59. Tihon J.: Flow Diagnostics in the Channel behind a Backward-Facing Step. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 48, Srní, Šumava, Czech Republic, 17-20 October 2005.
60. Tihon J., Pantzali M., Havlica J.: Flow Diagnostics in the Channel behind a Backward-Facing Step. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 166, Tatranské Matliare, Slovakia, 23-27 May 2005.
61. Večeř M., Bunganič R., Šimčík M., Růžička M., Drahoš J.: Local Gas Holdup Measurement in a Bubble Column: Optical Fiber Probe and Fast Video Camera. 7th Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Abstracts, p. 7.7., Strasbourg, France, 21-24 August 2005.
62. Večeř M., Bunganič R., Šimčík M., Růžička M., Drahoš J.: Experimentální studium lokální zadržky plynu v kapalině - optická sonda a ccd kamera. (Czech) Experimental Study of Local Gas Hold up by Optical Fibre Probe and CCD Camera. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 223, Srní, Šumava, Czech Republic, 17-20 October 2005.
63. Večeř M., Havlica J., Wein O., Punčochář M.: Koncové efekty při rotační viskozimetrii - experimenty a CFD simulace. (Czech) Edge Effects in Rotational Viscometry-Experiments and CFD Simulations. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 225, Srní, Šumava, Czech Republic, 17-20 October 2005.

64. Večeř M., Havlica J., Wein O., Punčochář M.: Edge Effects in Rotational Viscometry-Experiments and CFD Simulations. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 171, Tatranské Matliare, Slovakia, 23-27 May 2005.
65. Večeř M., Šimčík M., Růžička M., Drahoš J., Wichterle K.: A Case Study of Void Fraction Measurements Using Optical Probe. 43rd European Two-Phase Flow Group Meeting 2005, Program & List of Participants, Prague, Czech Republic, 11-13 May 2005.
66. Večeř M., Tovčigřečko V., Wein O.: AWS Viscometry of Polysaccharide Solutions Using a Novel KK Sensor. 2nd Annual Meeting European Society of Rheology AERC 2005, Abstracts, p. 144, Grenoble, France, 21-23 April 2005.
67. Večeř M., Wein O.: A Novel KK Sensor in AWS Viscometry of Polysaccharide Solutions. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 276, Tatranské Matliare, Slovakia, 23-27 May 2005.
68. Vejražka J., Cvetinovic D., Tihon J.: Control of Impinging Jets by Flow Excitation. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 170, Tatranské Matliare, Slovakia, 23-27 May 2005.
69. Vejražka J., Fujasová M., Stanovský P.: Spontánní tvorba bublin na jehle. (Czech) Spontaneous Bubble Production on the Needle. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 61, Srní, Šumava, Czech Republic, 17-20 October 2005.
70. Vejražka J., Stanovský P., Fujasová M.: Řízená tvorba bublin. (Czech) Controlled Production of Bubbles. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 60, Srní, Šumava, Czech Republic, 17-20 October 2005.
71. Wein O., Tovčigřečko V., Sobolík V.: Voltage-step Transient in Viscometric Flow under Apparent Wall Slip. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 231, Srní, Šumava, Czech Republic, 17-20 October 2005.
72. Wein O., Večeř M., Tovčigřečko V., Sobolík V.: Velocity Profiles in Depleted Layer of Aqueous Polymer Solutions. 2nd Annual Meeting European Society of Rheology AERC 2005, Abstracts, p. 134, Grenoble, France, 21-23 April 2005.
73. Wichterle K., Raška P., Kulhánková L., Růžička M.: Interakce stoupajících elipsoidálních bublin. (Czech) Hydrodynamic Interactions of Rising Ellipsoidal Bubbles. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 224, Srní, Šumava, Czech Republic, 17-20 October 2005.

Department of New Processes in Chemistry and Biotechnology

Head: J. Čermák
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Research staff: M. Czakóová, J. Hájek, G. Kuncová, Y. Maléterová, O. Podrazký, S. Šabata, L. Šťastná, J. Včelák
Part time: J. Hetflejš, F. Kaštánek
Technical staff: J. Brustman, A. Churavá, J. Kubešová, Z. Soukup, J. Žádný
PhD students: J. Bolyó, P. Gavlasová, A. Krupková, M. Pošta, J. Storch, J. Trögl

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
- New cyclization reaction affording dinitrogen heterocycles
- Generation of new compounds for blood substitutes and other biomedical applications

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

Microbial degradation of phenolic compounds in water and sediments

(F. Kaštánek, supported by GA CR, grant No.104/03/0407)

The screening and adaptation of selected strain *Pandoreae sp.* were carried out with the aim to degrade 4-chlorophenol. Immobilized cells on the carrier particles proved to be more effective compared to the submerged cell culture. The degradation of chlorophenols present in

real soils has to be solved according to a soil type using combined chemical and biodegradation procedure. [Refs. 17, 18, 38, 39]

Transformation of liquid polybutadienes to polymeric antidegradants and block copolymers

(J. Hetflejš, supported by GA CR grant No. 203/03/0617)

A series of di- and three-block butadiene-siloxane copolymers were prepared by several polymer analogous reactions using siloxanes with reactive end groups as Si-block precursors. The finding of the exclusive formation of *Z,Z*-dilithio-2-butene by interaction of Li with butadiene was used to propose a novel stereoselective synthesis of disilylated 2-butenes. [Ref. 22]

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. [Refs. 6, 35-37]

Microwave technology for production of new glasses

(M. Hájek, supported by GA ASCR, grant No. S4072003)

A new technology for melting and manufacture of glass has been applied for production of new kinds of glasses. [Refs. 26, 27, 43]

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. 2, 10, 29, 30]

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. 12]

Novel fluorophilic ligands for transition metal complexes based on polyfluorinated alkynes

(J. Čermák, supported by ICPF)

The synthetic pathways leading to a $[(C_5Me_4C_nF_{2n+1})M]$ ($M = Rh, Ir$) fragment were investigated, starting from Rh(III) phosphine and amine complexes or from Rh(I) alkene and diene complexes. The ability of novel heavily fluorinated cyclopentadienes substituted by four polyfluorinated chains to complex with selected transition metals was examined. [Ref. 31]

New catalysts based on diphosphinoazine complexes

(J. Čermák, supported by ICPF)

Nickel(II) complexes of diphosphinoazines were found to catalyze, together with MAO, ethylene polymerization. Thorough study of hydroamination of methyl methacrylate with various amines was carried out. The ability of some amines to react in the uncatalyzed reaction was revealed; the reaction catalyzed by diphosphinoazine palladium(II) complexes was investigated more in detail. Cycloocta-1,5-diene complexes of Rh(I) with diphosphinoazines were synthesized and characterized including X-ray diffraction. [Refs. 9, 21, 24, 32]

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 of yeast and mixed microbial culture for MTBE biodegradation. The basic parameters of the optical glucose sensor for bioreactors were determined: concentration range 0-3 mmol glucose /L, sensitivity 0.2 mmol glucose/L, response time <30 s. The glucose sensor performed stable measurement during one week cultivation of yeast.

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

G. Kuncova, Joint project with ICT, supported by GA CR, grant No. 104/05/2637

Microorganisms degrading MTBE obtained from ICT were cultivated in flasks and in laboratory bioreactors. In 5 L laboratory bioreactor were cultivated mixed MTBE degrading microbial cultures for 3 weeks and in 250 ml bubbled fixed bed reactor for 3 months. A sorption on porous minerals was tested as an alternative process of MTBE removal. The new route of preparation of polydimethylsiloxanes, perspective carriers for applications in biotechnologies was developed. [Ref. 13]

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

Pedro Vidinha, Universidade Nova de Lisboa, Lisbon, Portugal (1 week)

K. Tregubov, Universidad Central de Venezuela, Caracas, Venezuela

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. Betancor L., López-Gallego F., Hidalgo A., Fuentes M., Podrazký O., Kuncová G., Guisán J.M., Fernández-Lafuente R.: Advantages of the Pre-Immobilization of Enzymes on Porous Supports for Their Entrapment in Sol-Gels. *Biomacromolecules* 6(2), 1027-1030 (2005).
2. Církva V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry III. Photochemistry of 4-tert-Butylphenol. *J. Photochem. Photobiol., A* 174(1), 38-44 (2005).
3. Kaštánek F., Kaštánek P.: Combined Decontamination Processes for Wastes Containing PCBs. *J. Hazard. Mater.* 117(2-3), 185-205 (2005).
4. Paleček J., Církva V., Relich S., Slavětínská L., Kuča K., Jun D.: Přiřazení struktur reaktivátorů organofosfáty-inhibované acetylcholinesterázy na základě spekter nukleární magnetické rezonance. (Czech) The Structure Assignment of Reactivators of Organo-Phosphate Inhibited Acetylcholinesterase on the Basis of Nuclear Magnetic Resonance Spectra. *Zpravodaj vojenské farmacie* 15(1), 14-25 (2005).
5. Podrazký O., Kuncová G.: Determination of Concentration of Living Immobilized Yeast Cells by Fluorescence Spectroscopy. *Sens. Actuators, B* 107(1), 126-134 (2005).
6. Pyszková M., Lovás M., Jakabský Š., Hájek M.: The Application of Microwave Energy in Waste Technology. *Chem. Listy* 99, s90-s92 (2005).
7. Trögl J., Ripp S., Kuncová G., Saylor G.S., Churavá A., Pařík P., Demnerová K., Hálová J., Kubicová L.: Selectivity of Whole Cell Optical Biosensor with Immobilized Bioreporter *Pseudomonas Fluorescens* HK44. *Sens. Actuators, B* 107(1), 98-103 (2005).
8. Vlková L., Církva V.: Chlorované fenoly a způsoby jejich degradace. Chlorinated Phenols and Methods of Their Degradation. *Chem. Listy* 99(2), 125-130 (2005).
9. Carvalho M.F., Čermák Jan, Fernandes A.C., Ferreira A.S., Galvao A.M., Matos I., Marques M.M.: Cationic Ni-Diphosphine Azine Complexes as Catalysts for Ethylene Polymerisation. *Inorg. Chim. Acta*, submitted.
10. Církva V., Vlková L., Relich S., Hájek M.: Microwave Photochemistry IV: Preparation of the Electrodeless Discharge Lamps for Photochemical Applications. *J. Photochem. Photobiol., A*, in press.
11. Gavlasová P., Kuncová G., Macková M.: Approaches to Design Whole Cell Biosensors for PCB Analysis Based on Optical Detection. *Biodegradation*, submitted.
12. Hájek M.: Microwave Drying of Paper Documents. *Ceram. Trans.*, submitted.
13. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus J.: Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.*, in press.
14. Hetflejš J., Šabata S., Podešva J., Netopilík M., Látalová P., Spěváček J.: Synthesis of Triblock Polybutadiene-Poly-(dimethylsiloxane) Copolymers by Coupling Reactions. *J. Appl. Polym. Sci.*, submitted.
15. Kaštánek F.: System of Decontamination of Wastes Containing PCBs. *J. Hazard. Mater.*, in press.
16. Kaštánek F., Hanika J.: Úloha chemického inženýrství ve zvyšování bezpečnosti chemických výrob. (Czech) The Role of Chemical Engineering in Chemical Process Safety. *Chem. Listy*, 100, 150-155 (2006).

17. 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.
18. Kaštánek F., Maléterová Y., Kaštánek P., Rott J., Jiříčný V., Jirátová K.: Complex Treatment of Soils, Waste Water and Groundwater Contaminated by Halogenated Organic Compounds. Desalination, in press.
19. Kaštánek F., Páca J., Maléterová Y.: Biodegradation of Phenol at the Presence of Polyaromatic Hydrocarbons (PAH) in Soil. Int. Biodeterior. Biodegrad., submitted.
20. Leitmannová E., Storch J., Červený L.: Selective Two-Phase Hydrogenations of Sorbic Acid Using [Cp**Ru*(sorbic acid)]⁺ Catalyst. *Reac. Kinet. Catal. Lett.*, submitted.
21. Pošta M., Čermák Jan, Vojtíšek P., Císařová I.: Diphosphinoazine Rhodium(I) and Iridium(I) Complexes. *Collect. Czech. Chem. Commun.*, in press.
22. Šabata S., Blechta V., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. *J. Organomet. Chem.*, submitted.
23. 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. *Sens. Actuators, B*, submitted.
24. Včelák J., Čermák Jan, Czakoová M., Storch J.: Hydroamination of Methyl Methacrylate Catalyzed by Cationic Palladium Diphosphinoazine Complexes. *Tetrahedron*, submitted.

Review papers

25. Gavlasová P., Kuncová G., Macková M.: Stanovení PCB - Chemické versus biologické metody. (Czech) Determination of PCBs - Chemical Versus Biological Methods. *Biol. listy* 70(3), 211-230 (2005).

Patents

26. Hájek M., Drahoš J., Volf V., Vozáb J.: Method and Apparatus for Heat Treatment of Glass Material and Natural Materials Specifically of Volcanic Origin. Pat. No. 6,938,441 B1/10/018,119. Applied: 00.06.12, Patented: 05.09.06.
27. Hájek M., Drahoš J., Volf V., Vozáb J.: Sposob a zariadenie na tepelné zpracovanie 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. 284 512/1690-2001. Applied: 00.06.12, Patented: 05.05.05.

Conferences

28. Blechta V., Sýkora J., Hetflejš J., Šabata S., Schraml J.: LC-NMR of Organosilicon Polymers with Indirect ²⁹Si NMR Detection for Polymer Identification. 14th International Symposium on Organosilicon Chemistry ISOSXIV, Program, Abstracts, and List of Participants, p. P 184, Würzburg, Germany, 31 July - 05 August 2005.
29. Církva V.: Microwave Photochemistry. 1st Avogadro Symposium Quo Vadis Chemistry?, Sorisole, Italy, 09-11 September 2005.
30. Církva V., Relich S., Vlková L., Hájek M.: Microwave Photochemistry: Preparation of the Electrodeless Discharge Lamps and Their Photochemical Applications. 10th International Conference on Microwave and High Frequency Heating, Proceedings Book, p. 183-186, Modena, Italy, 12-15 September 2005.
31. Čermák Jan, Auerová K., Bříza T., Šťastná L., Kvíčala J.: Cyclopentadienes and Cyclopentadienyl Complexes with Fluorous Ponytails. XVIth FECHEM Conference on Organometallic Chemistry, Book of Abstracts, p. 28, Budapest, Hungary, 03-08 September 2005.
32. Čermák Jan, Včelák J., Czakoová M., Storch J.: Hydroamination of Methyl Methacrylate Catalyzed by Cationic Palladium Diphosphinoazine Complexes. XVIth FECHEM Conference on Organometallic Chemistry, Book of Abstracts, p. 95, Budapest, Hungary, 03-08 September 2005.

33. Čertík M., Bolyó J., Dodok L.: Aplikácia polosuchých kultivácií pri príprave cereálnych výrobkov obohatených o polynenasýtené mastné kyseliny. (Slov) Application of Solid State Fermentation for Preparing Cereal Goods Enriched by Polyunsaturated Fatty Acids. 7. zjazd Slovenskej spoločnosti pre poľnohospodárske, lesnícke, potravinárske a veterinárne vedy pri SAV, Zborník prednášok, p. 44-49, Bratislava, Slovakia, 08 September 2005.
34. Dodok L., Bolyó J., Čertík M.: Vplyv prídavku fermentačných produktov obsahujúcich kyselinu gamma-linolénovú na reologické vlastnosti cesta a cereálnych výrobkov. (Slov) Effect of Addition of Fermentation Products Containing gamma-Linolenic Acid into Rheological Properties of the Dough and Cereal Goods. 7. zjazd Slovenskej spoločnosti pre poľnohospodárske, lesnícke, potravinárske a veterinárne vedy pri SAV, Zborník prednášok, p. 142-146, Bratislava, Slovakia, 08 September 2005.
35. Hájek M.: Simultaneous Cooling in Microwave Synthesis. 1st Avogadro Symposium Quo Vadis Microwave Chemistry?, Sorisole, Italy, 09-11 September 2005.
36. Hájek M., Kurfürstová J.: Microwave Effects in Heterogeneous Catalysis. 10th International Conference on Microwave and High Frequency Heating, Proceedings Book, p. 150-154, Modena, Italy, 12-15 September 2005.
37. Hájek M., Kurfürstová J.: Microwave Effects in Heterogeneous Catalysis. 14 Congreso Científico internacional Simposio: Tecnologías de microondas: Aplicaciones en Química y Biología, Programme de Actividades, p. 92 (T17), Habana, Cuba, 27-30 June 2005.
38. Kaštánek F., Kaštánek P., Maléterová Y., Rott J.: Are Available Safety Methods for Degradation of Hazardous Polyhalogenated Wastes (Containing PBDEs, PCBs)? 18 Conferencia internacional de química, Santiago de Cuba, Cuba, 06-09 December 2005.
39. Kaštánek F., Maléterová Y., Kaštánek P., Rott J.: Complex Treatment of Soils, Waste Water and Groundwater Contaminated by Halogenated Organic Compounds. 9th International Conference on Environmental Science and Technology, Proceedings, p. 112, Rhodes Island, Greece, 01-03 September 2005.
40. Kuncová G., Bolyó J., Podrazký O.: Yeast Cells Entrapped in Silica and Silica-Alginate Matrix. 13th International Workshop on Sol-Gel Science and Technology, Abstracts and Program, p. 1-2, Los Angeles, USA, 21-26 August 2005.
41. Müller P., Klán P., Literák J., Církva V.: Application of Microwave-Assisted Photochemistry. 8th International Conference on Solar Energy and Applied Photochemistry Solar'05, Book of Abstracts, p. 92-93, Luxor, Egypt, 20-25 February 2005.
42. Pyszková M., Lovás M., Jakabský Š., Hájek M.: The Mechanical Properties of Microwave Vitrification Waste. 9th Conference on Environment and Mineral Processing Part II, Proceedings, p. 25-28, Ostrava, Czech Republic, 23-25 June 2005.

Environmental Process Engineering Laboratory

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PhD students: P. Hejdová, M. Pohořelý, S. Relich, M. Šyc, M. Vosecký

Fields of research

- Persistent organic pollutants
- Gas-solid reactions
- 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

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

(M. Punčochář, supported by EUREKA 1P04OE156)

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. On the laboratory scale experiments were found the conditions for the formation of highly chlorinated PCDDs, which have the same atypical fingerprint as compared with non-anthropogenic PCDD. The solution of optimization of combustion conditions in Liberec MSW incinerator was directed to ammonia concentration reduction after non-catalytic NO_x destruction technology. [Refs. 9, 24, 30]

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. Physicochemical characteristics of a series of materials suitable as biofuels have been determined. Special attention is paid to the process leading to the lowering of emissions of persistent organic pollutants, heavy metals, HCl, and NO_x. [Refs. 6, 18, 20, 28, 37]

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. 2, 7, 12-15, 17, 19, 32]

Preparation of electrodeless lamp for photochemical applications

(V. Církva, supported by ICPF)

The project is concerning on preparation of the electrodeless discharge lamps (EDLs) as a suitable source of UV/VIS light for photochemical reactions. The effect of operating EDL parameters, the microwave power output and medium properties on spectral characteristics are studied. [Refs. 1, 11, 25, 26, 29]

International co-operations

Vrije Universiteit Brussels, Brussels, Belgium: Formation of POPs

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

Visits abroad

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

Publications

Original papers

1. Církva V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry III. Photochemistry of 4-tert-Butylphenol. J. Photochem. Photobiol., A 174(1), 38-44 (2005).

2. Hartman M., Svoboda K., Pohořelý M., Trnka O.: Combustion of Dried Sewage Sludge in a Fluidized-Bed Reactor. *Ind. Eng. Chem. Res.* 44(10), 3432-3441 (2005).
3. Hartman M., Trnka O., Šolcová O.: Thermal Decomposition of Aluminium Chloride Hexahydrate. *Ind. Eng. Chem. Res.* 44(17), 6591-6598 (2005).
4. Kušar H.M.J., Ersson A.G., Vosecký M., Järås S.G.: Selective Catalytic Oxidation of NH₃ to N₂ for Catalytic Combustion of Low Heating Value Gas under Lean/Rich Conditions. *Appl. Catal., B* 58(1-2), 25-32 (2005).
5. Paleček J., Církva V., Relich S., Slavětínská L., Kuča K., Jun D.: Přiřazení struktur reaktivátorů organofosfáty-inhibované acetylcholinesterázy na základě spekter nukleární magnetické rezonance. (Czech) The Structure Assignment of Reactivators of Organo-Phosphate Inhibited Acetylcholinesterase on the Basis of Nuclear Magnetic Resonance Spectra. *Zpravodaj vojenské farmacie* 15(1), 14-25 (2005).
6. Punčochář M., Drahoš J.: Origin of Pressure Fluctuations in Fluidized Beds. *Chem. Eng. Sci.* 60(5), 1193-1197 (2005).
7. Trnka O., Hartman M., Veselý V.: Charakteristika tlakových fluktuací v různých režimech suspenzí plyn - tuhá látka. (Czech) Characteristics of the Pressure Fluctuations in Different Operation Regimes of Gas-Solid Suspensions. *Chem. Listy* 99(5), 330-338 (2005).
8. Tydlitát V., Pekárek V., Janota J., Kotlík B., Sysalová J.: Složení tuhé znečišťující látky z ovzduší v blízkosti pražské dopravní tepny. (Czech) Composition of the Suspended Particular Matter in the Atmosphere near of a Prague Traffic Artery. *Ochrana ovzduší* 17(37)(3), 5-6 (2005).
9. Vlková L., Církva V.: Chlorované fenoly a způsoby jejich degradace. (Czech) Chlorinated Phenols and Methods of Their Degradation. *Chem. Listy* 99(2), 125-130 (2005).
10. 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).
11. Církva V., Vlková L., Relich S., Hájek M.: Microwave Photochemistry IV: Preparation of the Electrodeless Discharge Lamps for Photochemical Applications. *J. Photochem. Photobiol., A*, in press.
12. Hartman M.: Letter to the Editor. Three-dimensional Modeling of a Circulating Fluidized-Bed Gasifier for Sewage Sludge. *Chem. Eng. Sci.*, in press.
13. 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*, in press.
14. Hartman M., Pohořelý M., Trnka O.: Fluidization of Dried Wastewater Sludge. *Powder Technol.*, submitted.
15. Hartman M., Pohořelý M., Trnka O.: Transport Velocities of Different Particulate Materials in Pneumatic Conveying. *Chem. Pap.*, in press.
16. Hartman M., Trnka O.: Comments on "Ceria-Zirconia High-Temperature Desulfurization Sorbents". *Ind. Eng. Chem. Res.*, submitted.
17. 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. *Energetika*, submitted.
18. Pekárek V., Punčochář M., Bureš M., Grabic R., Fišerová E.: Effect of Sulfur Dioxide, Hydrogen Peroxide and Sulfuric Acid on the De novo Synthesis of PCDD/F and PCB in the N₂ + 10 % O₂ Atmosphere under Model Laboratory Conditions. *Chemosphere*, submitted.
19. Pohořelý M., Svoboda K., Trnka O., Baxter D., Hartman M.: Gaseous Emissions from the Fluidized-bed Incineration of Sewage Sludge. *Chem. Pap.*, in press.
20. Pohořelý M., Vosecký M., Hejdrová P., Punčochář M., Skoblia S., Staf M., Vošta J., Koutský B., Svoboda K.: Gasification of Coal and Plastic Waste in Fluidized Bed Reactor. *Fuel*, submitted.
21. Schwarz J., Smolík J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate Emissions from Fluidized Bed Combustion with Fly Ash Recirculation of Czech Lignite with and without Calcareous Additives. *Fuel Process. Technol.*, submitted.

Review papers

22. Fernandez-Gutierrez M.-J., Baxter D., Hunter Ch., Svoboda K.: Nitrous Oxide (N₂O) Emissions from Waste and Biomass to Energy Plants. *Waste Manage. Res.* 23(2), 133-147 (2005).

Conferences

23. Brechler J., Pekárek V., Tydlitát V., Janota J.: Případová studie rozptylu par rtuti z bodového zdroje. (Czech) Case Study of Mercury Dispersion from Point Source. *Ovzduší 2005*, Program a Sborník konference, p. 83-86, Brno, Czech Republic, 09-11 May 2005.
24. Bureš M., Pekárek V.: Dehalogenace polychlorovaných bifenyly. (Czech) Dehalogenation of Polychlorinated Biphenyls. 27. Mezinárodní slovenský a český kalorimetrický seminář 2005, Sborník příspěvků, p. 45-48, Svatka, Czech Republic, 23-27 May 2005.
25. Církva V.: Microwave Photochemistry. 1st Avogadro Symposium Quo Vadis Chemistry?, Sorisole, Italy, 09-11 September 2005.
26. Církva V., Relich S., Vlková L., Hájek M.: Microwave Photochemistry: Preparation of the Electrodeless Discharge Lamps and Their Photochemical Applications. 10th International Conference on Microwave and High Frequency Heating, Proceedings Book, p. 183-186, Modena, Italy, 12-15 September 2005.
27. Gruber V., Punčochář M.: Hydrometalurgické metody recyklace elektrotechnických odpadů. (Czech) Hydrometallurgical Methods of Recycling of Electronic Waste. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 105, Srní, Šumava, Czech Republic, 17-20 October 2005.
28. Hejdová P., Solich M., Vosecký M., Malecha J., Koutský B., Punčochář M., Skoblia S.: Zplyňování biomasy a vysokoteplotní čištění plynu. (Czech) Biomass Gasification and High Temperature Gas Cleaning. New Trends in Technology Systems Operation'05, Book of Abstracts, p. 221-224, Prešov, Slovakia, 20-21 November 2005.
29. Müller P., Klán P., Literák J., Církva V.: Application of Microwave-Assisted Photochemistry. 8th International Conference on Solar Energy and Applied Photochemistry Solar'05, Book of Abstracts, p. 92-93, Luxor, Egypt, 20-25 February 2005.
30. Pekárek V., Ocelka T., Grabic R.: The Application of CMD Method for Destruction of Chlorinated Pesticides and Some Pre-Dioxin and POP Compounds. Environmentally Sound Management Practices on Cleaning Up Obsolete Stockpiles of Pesticides for Central European and EECCA Countries, Abstracts, p. 39, Sofia, Bulgaria, 26-28 May 2005.
31. Pohořelý M., Svoboda K., Hejdová P., Vosecký M., Trnka O., Hartman M.: Spalování velmi mokrych stabilizovaných čistírenských kalů v atmosferickém fluidním reaktoru. (Czech) Combustion of Wet Sewage Sludge in Atmospheric Fluidized Bed Reactor. 57. zjazd chemických spoločností, ChemZi, p. 6Po14, Tatranské Matliare, Slovakia, 04-08 September 2005.
32. Pohořelý M., Svoboda K., Trnka O., Hartman M.: Gaseous Emissions from the Fluidized-bed Incineration of Sewage Sludge. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 82, Tatranské Matliare, Slovakia, 23-27 May 2005.
33. Punčochář M., Veselý V.: Chemická recyklace PET lahví. (Czech) Chemical Recycling PET Bottles. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 106-107, Srní, Šumava, Czech Republic, 17-20 October 2005.
34. Svoboda K., Pohořelý M., Martinec J., Baxter D., Hunter Ch.: Integration of Biomass Drying with Combustion/Gasification Technologies and Minimization of Emissions of Organic Compounds. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 51, Tatranské Matliare, Slovakia, 23-27 May 2005.
35. Večeř M., Havlica J., Wein O., Punčochář M.: Edge Effects in Rotational Viscometry-Experiments and CFD Simulations. 32nd International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 171, Tatranské Matliare, Slovakia, 23-27 May 2005.
36. Večeř M., Havlica J., Wein O., Punčochář M.: Koncové efekty při rotační viskozometrii - experimenty a CDF simulace. (Czech) Edge Effects in Rotational Viscometry-Experiments and CFD Simulations. 52. Konference chemického a procesního inženýrství CHISA 2005, Sborník 1, p. 225, Srní, Šumava, Czech Republic, 17-20 October 2005.

37. Vosecký M., Skoblia S., Koutský B., Malecha J., Punčochář M.: Gazifikatsiya biomassy i ee perspektivy dlya proizvodstva elektricheskoi energii. (Russ) Biomass Gasification and Perspectives of Its Utilization in Electricity Production. Mezhdunarodnaya nauchno-tekhnicheskaya konferentsiya "Resursno- i energosberegayushchie tekhnologii i oborudovanie, ekologicheski bezopasnye tekhnologii", Materialy konferentsii, p. 72-78, Minsk, Belarus, 16-18 November 2005.

Laboratory of Aerosol Chemistry and Physics

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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

Integrated exposure management tool characterizing air pollution – relevant human exposure in urban environment

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

The objective of the project is to study human exposure from air-pollution compounds that account for two important pathways exposure (inhalation and dermal absorption), and to quantify exposure specifically for particulate matter and chloroform in several European urban areas. The scientific aim is to develop science-based methods for quantification of exposure. The environmental and policy-relevant product is the implementation of these methods in conjunction with a robust multiphase modelling environmental management system. [Refs. 2, 20, 26]

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 are compared to the results obtained from measurements in real indoor environment (indoor living space). [Refs. 2, 6, 16, 20, 23, 34-37]

Contribution of secondary atmospheric PM to total PM pollution loading

(J. Smolík, supported by Ministry of Environment CR, 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 will be performed with subsequent gravimetric and chemical analyses. The contribution of the inorganic part will be determined using ion chromatography.

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.

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 will be used to find the limits of stability and CFD methods will be 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, 4, 13, 17, 18, 24, 27, 28, 38]

Comprehensive size resolved characterization of atmospheric particulate matter in Prague

(J. Schwarz, supported by GA CR, grant No. 205/03/1560)

The goal of the project is comprehensive characterization of atmospheric aerosol in Prague. For this purpose concurrent sampling on two sites is performed using cascade impactors, SMPS systems, nano-SMPS and APS together with filter based sampling, yielding particle mass and number size distributions. The relations between size and composition are studied using PIXE, PIGE, INAA, ICP-MS, IC, AAS, and GC-MS analyses. The data together with the available source fingerprints are used in main aerosol sources identification. Further, the relation between aerosol mass and particle number size distributions and composition and atmospheric conditions is also analysed. The project is solved in collaboration with Charles University, Prague and Nuclear Physics Institute AS CR. [Refs. 21, 22, 31-36, 40]

Nucleation studies using diffusion chambers. Atmospheric aerosol measurements - instruments intercomparison

(V. Ždímal, supported by Ministry of Education, grant No. ME 699, program KONTAKT)

This bilateral (Czech-Greek) project solves two tasks. First one is focused on modelling. Its aim is to improve a model describing the coupled mass, heat and momentum transport inside the flow diffusion chamber. The CFD approach using the code FLUENT will be used to accomplish this task and to evaluate the experimental data. The second task is to perform an comparison of two instruments measuring particle size distributions, the SMPS system and LAS-X, based on different physical principles. An aerosol generator will be used producing a

monodisperse aerosol and this aerosol will be led into both devices at the same time. The whole available size range will be studied. [Refs. 1, 17-19]

Light-induced nucleation from supersaturated vapors

(V. Ždímal, supported by NATO, grant No. PST.CLG.979351)

The aim of this cooperative linkage project is fundamental and applied research in the field of homogeneous and light-induced nucleation. A new experimental technique will be used, developed especially for the investigations of light-induced nucleation in the diffusion cloud chamber. Substances showing very intriguing properties, e.g. sulphur, will be studied. The very complex phase behaviour of sulphur will be taken into account including its tendency to form stable oligomers in the vapour phase, and the presence of so called lambda point at which many physical properties of sulphur change dramatically.

Metastable water and steam

(V. Ždímal, supported by GA CR, grant No. 101/05/2214/1)

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 will be carried out. A device will be developed for measurement of the surface tension of supercooled water. Studies on homogeneous nucleation from supercooled water vapor will 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 will be studied. Water clusters, bulk supercooled liquid and its surface will be simulated using Monte Carlo and molecular dynamics. Based on both experimental and simulation results, semi-phenomenological analytical models of metastable water and water clusters will be developed, enabling engineering application.

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 will be 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 will be developed to connect these devices, operating at laboratory conditions, to sampling ports of the turbine at high pressure and temperature. Experiments will be carried out in laboratories and subsequently in a power plant. The results will be compared with measured structure of the developed liquid phase, which depends on heterogeneous condensation nuclei, and with theoretical analysis. [Ref. 25]

International co-operations

Philipps-University Marburg, Marburg, Germany: Experimental study of homogeneous nucleation in supersaturated vapours

Finnish Meteorological Institute, Helsinki, Finland: Application of cascade impactors for aerosol studies; 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
Johns Hopkins University, Baltimore, USA: Light-induced nucleation from supersaturated vapors
Institute of Physical Chemistry Russian Academy of Sciences, Moscow, Russia: Non-equilibrium phenomena on the solid-gas boundary
Karpov Institute of Physical Chemistry, Aerosol Department, Moscow, Russia: Nucleation processes studied in diffusion chambers
Ghent University, Institute for Nuclear Sciences, B-9000 Ghent, Belgium: OC/EC in urban and suburban PM10 aerosol in Prague

Visitors

H. Keskinen, Institute of Physics, Tampere University of Technology, Tampere, Finland
H. Uchtmann, Philipps-University Marburg, Marburg, Germany
C. Housiadas, Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece
B. Finnlayson-Pitts a J. Pitts, University of California Irvine, U.S.A.
R. Hillamo, Finnish Meteorological Institute, Helsinki, Finland

Publications

Original papers

1. Brus D., Hyvärinen A.-P., Ždímal V., Lihavainen H.: Homogeneous Nucleation Rate Measurements of 1-Butanol in Helium: A Comparative Study of a Thermal Diffusion Cloud Chamber and a Laminar Flow Diffusion Chamber. *J. Chem. Phys.* 122(21), 214506 (2005).
2. Coulson G., Bartonova A., Böhler T., Broday D.M., Colbeck I., Fløisand I., Fudala J., Hollander W., Housiadas Ch., Lazaridis M., Smolík J.: Exposure Risks from Pollutants in Domestic Environments: The Urban Exposure Project. *Indoor Built Environ.* 14(3-4), 209-213 (2005).
3. Levdansky V.V., Smolík J., Moravec P.: Critical Size of Aerosol Particles in the Resonance Radiation Field. *Int. Commun. Heat Mass Transfer* 32(1-2), 116-122 (2005).
4. Levdansky V.V., Smolík J., Moravec P.: Vliyaniye poverkhnostnykh protsessov i vneshnikh polei na yavleniya perenosa i fazovye perekhody v aerol'nykh sistemakh s nanorazmernymi chastitsami. (Russ) Influence of Surface Processes and External Fields on Transfer Phenomena and Phase Transitions in Aerosol Systems with Nanosize Particles. *Inzh.-Fiz. Zh. (J. Eng. Phys. Thermophys.* 78(1), 104-108) 78(1), 101-105 (2005).
5. Moravec P., Smolík J., Levdansky V.V.: Preparation of Al₂O₃-SiO₂ Fine Particles by CVD Method in Tube Flow Reactor. *Powder Technol.* 153(3), 159-165 (2005).
6. Smolík J., Lazaridis M., Moravec P., Schwarz J., Zaripov S.K., Ždímal V.: Indoor Aerosol Particle Deposition in an Empty Office. *Water, Air, Soil Pollut.* 165, 301-312 (2005).

7. Bryant C., Eleftheriadis K., Smolík J., Ždímal V., Mihalopoulos N., Colbeck I.: Optical Properties of Aerosols over the Eastern Mediterranean. *Atmos. Environ.*, in press.
8. 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.*, submitted.
9. 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.*, in press.
10. Levdansky V.V., Smolík J., Moravec P.: Vliaynie poverkhnostnykh effektov pri kondenzatsii para na nanorazmernoi chastitse imeyuschei elektricheskii zaryad. (Russ) Influence of Surface Effects in Vapor Condensation on Nanoscale Particle with Electric Charge. *Inzh. - Fiz. Zh. (J. Eng. Phys. Thermophys.)*, submitted.
11. Levdansky V.V., Smolík J., Moravec P.: Free Molecule Flow of Gases in Channels (Pores) in Physico-Chemical Transformation on Surface. *Int. J. Heat Mass Transfer*, submitted.
12. Levdansky V.V., Smolík J., Moravec P.: Vliyanie razmernykh effektov na kriticheskii diametr i skorost' rosta nanochastits. (Russ) Influence of Size Effects on Critical Diameter and Growth Rate of Nanoparticles. *Inzh. - Fiz. Zh.*, submitted.
13. Levdansky V.V., Smolík J., Moravec P.: Influence of Size Effect and Foreign Gases on Formation of Nanoparticles. *Int. Commun. Heat Mass Transfer*, 33, 56-60 (2006).
14. 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.
15. Schwarz J., Smolík J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate Emissions from Fluidized Bed Combustion with Fly Ash Recirculation of Czech Lignite with and without Calcareous Additives. *Fuel Process. Technol.*, submitted.

Conferences

16. Barták M., Smolík J., Dohányosová P.: Softwarový modul Urban Exposure pro hodnocení účinků škodlivin v ovzduší. (Czech) The Urban Exposure Management Tool for Assessment of Exposure of Residents to Urban Air Pollution. *Konference Ovzduší 2005, Program a sborník konference*, p. 232-233, Brno, Czech Republic, 09-11 May 2005.
17. Brus D., Hyvärinen A.-P., Ždímal V., Lihavainen H.: Comparison Homogeneous Nucleation Rate Measurements of 1-Butanol-Helium System in Diffusion Chambers. *32nd International Conference of Slovak Society of Chemical Engineering, Proceedings*, p. 279, Tatranské Matliare, Slovakia, 23-27 May 2005.
18. Brus D., Hyvärinen A.-P., Ždímal V., Lihavainen H.: A Comparison Study: Homogeneous Nucleation of n-Butanol in Helium, using a Thermal Diffusion Cloud Chamber and a Laminar Flow Diffusion Chamber. *European Aerosol Conference EAC 2005, Book of Abstracts*, p. 36, Ghent, Belgium, 28 August - 02 September 2005.
19. Eleftheriadis K., Ždímal V., Wagner Z., Vratolis S.: Performance Comparison of SMPS and LAS-X using Ammonium Sulphate and Sodium Chloride Aerosol. *European Aerosol Conference EAC 2005, Book of Abstracts*, p. 297, Ghent, Belgium, 28 August - 02 September 2005.
20. Glytsos T., Aleksandropoulos V., Smolík J., Lazaridis M.: Estimating the Strength of Indoor Sources using a Comprehensive Microenvironmental Model. *European Aerosol Conference EAC 2005, Book of Abstracts*, p. 533, Ghent, Belgium, 28 August - 02 September 2005.
21. Hovorka J., Braniš M., Schwarz J.: Diurnal Variation of Submicron PM Size Distribution and Gaseous Pollutant Concentration during a Year 2004 in Prague, *Pollution Source Estimation. Particulate Matter Supersites Program & Related Studies 2005 AAAR, Abstracts*, p. 77, Atlanta, GA, USA, 07-11 February 2005.
22. Hovorka J., Braniš M., Schwarz J.: Diurnal Pattern of Submicron Aerosol Size/Mass Distributions in Urban Atmosphere, Prague Winter 2004/2005. *European Aerosol Conference EAC 2005, Book of Abstracts*, p. 619, Ghent, Belgium, 28 August - 02 September 2005.

23. Hruška A., Dohányosová P., Hemerka J., Smolík J.: Depozice aerosolů ve vnitřním prostředí. Aerosol Deposition in the Indoor Environment. VI. konference České aerosolové společnosti, Sborník konference, p. 15-18, Praha, Czech Republic, 15 November 2005.
24. Hyvärinen A.-P., Brus D., Lihavainen H., Ždímal V., Uchtmann H.: Homogeneous Nucleation of n-Butanol: The Carrier Gas Pressure Effect. European Aerosol Conference EAC 2005, Book of Abstracts, p. 583, Ghent, Belgium, 28 August - 02 September 2005.
25. Kolovratník M., Hrubý J., Ždímal V.: Aerosoly v parních turbínách?. (Czech) Aerosols in Steam Turbines?. VI. konference České aerosolové společnosti, Sborník konference, p. 37-41, Praha, Czech Republic, 15 November 2005.
26. Lazaridis M., Aleksandropoulos V., Smolík J., Glytsos T., Katsivela E., Dahlin E.: Indoor/Outdoor Particulate Matter Physicochemical Characteristics in Two Residential Houses. European Aerosol Conference EAC 2005, Book of Abstracts, p. 254, Ghent, Belgium, 28 August - 02 September 2005.
27. Levdansky V.V., Smolík J., Moravec P.: Size Effect in Aerosol Particle Formation. European Aerosol Conference EAC 2005, Book of Abstracts, p. 585, Ghent, Belgium, 28 August - 02 September 2005.
28. Levdansky V.V., Smolík J., Moravec P.: Size Effect in Formation of Nanoscale Particles by Deposition from Gas Phase. E-MRS 2005 Spring Meeting Current Trends in Nanoscience from Materials to Applications, Symposium A, p. A-22/22 - A-23/23, Strasbourg, France, 31 May - 03 June 2005.
29. Moravec P., Smolík J., Levdansky V.V., Keskinen H., Mäkelä J.M.: Production of Composite ZrO₂-SiO₂ Fine Particles by Thermal Decomposition of Zirconium Tetra-tert-butoxide and Tetraethyl Orthosilicate in an Externally Heated Tube Reactor. VI. konference České aerosolové společnosti, Sborník Konference, p. 27-30, Praha, Czech Republic, 15 November 2005.
30. Moravec P., Smolík J., Levdansky V.V., Keskinen H., Mäkelä J.M.: ZrO₂-SiO₂ Fine Particle Formation in an Externally Heated Tube Reactor by CVD Method. European Aerosol Conference EAC 2005, Book of Abstracts, p. 728, Ghent, Belgium, 28 August - 02 September 2005.
31. Schwarz J., Hovorka J., Ždímal V., Smolík J.: Mass Size Distribution of Prague Aerosol on Two Sites and during Three Seasons. European Aerosol Conference EAC 2005, Book of Abstracts, p. 712, Ghent, Belgium, 28 August - 02 September 2005.
32. Schwarz J., Smolík J., Hovorka J.: Studium velikostních distribucí atmosférických aerosolů vážených hmotou na předměstí Prahy. (Czech) Study of Atmospheric Aerosol Mass Size Distribution at Prague Suburb. Konference Ovzduší 2005, Program a sborník konference, p. 178-181, Brno, Czech Republic, 09-11 May 2005.
33. Schwarz J., Smolík J., Hovorka J., Civiš M.: Srovnání velikostních distribucí atmosférických aerosolů na pozadových stanicích v centru a na severozápadním předměstí Prahy. (Czech) The Comparison of Atmospheric Aerosol Mass Size Distributions at Urban Background Sites at Downtown and Northern-West Suburban of Prague. VI. konference České aerosolové společnosti, Sborník konference, p. 19-22, Praha, Czech Republic, 15 November 2005.
34. Smolík J., Schwarz J., Ždímal V., Dohányosová P.: Charakterizace aerosolů ve vnitřním prostředí. (Czech) Aerosol Characterization in the Indoor Environment. VI. konference České aerosolové společnosti, Sborník konference, p. 11-12, Praha, Czech Republic, 15 November 2005.
35. Smolík J., Schwarz J., Ždímal V., Lazaridis M., Dohányosová P.: Chemical and Elemental Size Distribution of Indoor/Outdoor Aerosol in Suburban Area of Prague. European Aerosol Conference EAC 2005, Book of Abstracts, p. 89, Ghent, Belgium, 28 August - 02 September 2005.
36. Smolík J., Schwarz J., Ždímal V., Lazaridis M., Dohányosová P.: Chemické složení vnitřního a venkovního aerosolu na předměstí Prahy. (Czech) Chemical Composition of Indoor and Outdoor Aerosol in Prague Suburb. Konference Ovzduší 2005, Program a sborník konference, p. 151-152, Brno, Czech Republic, 09-11 May 2005.
37. Smolík J., Schwarz J., Ždímal V., Lazaridis M., Dohányosová P.: Chování vnitřního aerosolu při běžných domácích činnostech. (Czech) Behaviour of Indoor Aerosol during Common Home

- Activities. Konference Ovzduší 2005, Program a Sborník konference, p. 147-150, Brno, Czech Republic, 09-11 May 2005.
38. Ždímal V., Brus D.: Vliv nosného plynu na kinetiku homogenní nukleace. Experimenty v přesycených parách 1-propanolu v heliu. (Czech) The Influence of the Carrier Gas on the Homogeneous Nucleation Kinetics. Experiments in Supersaturated Vapors of 1-Propanol in Helium. VI. konference České aerosolové společnosti, Sborník konference, p. 47-50, Praha, Czech Republic, 15 November 2005.
 39. Ždímal V., Moravec P., Smolík J., Mikuška P., Večeřa Z., Pokorný R.: Dynamika početních rozdělení velikostí aerosolových částic při experimentální kampani na stanici Bílý Kříž. (Czech) Dynamics of Aerosol Number Size Distributions during an Experimental Campaign at the Bily Kriz Measuring Site. Konference Ovzduší 2005, Program a sborník konference, p. 182-185, Brno, Czech Republic, 09-11 May 2005.
 40. Ždímal V., Schwarz J., Wagner Z., Dohányosová P., Smolík J.: The Dynamic of Atmospheric Aerosol Number Size Distributions at a Suburban Site in Prague. European Aerosol Conference EAC 2005, Book of Abstracts, p. 713, Ghent, Belgium, 28 August - 02 September 2005.

Laboratory of Laser Chemistry

Head: J. Pola
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Technical staff: D. Bártlová
PhD student: J. Blazevska-Gilev

Fields of research

- IR 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

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)

IR laser degradation of poly(vinyl acetate) was revealed as a specific process involving several novel decomposition paths (including formation of vinyl acetate) and allowing deposition of crosslinked polar polymeric films [Refs. 1, 8]. IR laser ablative decomposition of poly(vinyl acetate) loaded with metal nano- and micro-sized particles affords deposition of composites in which metal particles are embedded in polar crosslinked polymer films [Ref. 17]. IR laser ablative decomposition of poly(vinyl chloride) results in deposition of crosslinked polymer films containing less Cl than initial polymer [Ref. 16]. IR laser ablative decomposition of poly(1,4-phenylene sulphide) allows deposition of polymers with very low sulphur content and has been established to have potential for desulfurization of polyaromatic substances [Ref. 5]. Both laser degradations of the poly(vinyls) represent a novel mode of fabrication of polar intractable polymeric films and they are unique processes for degradation of poly(vinyls) into the monomer. In the first study on thermal stability of nanocomposite core-shell materials, thermogravimetric analysis of laser-prepared nano Fe/organosilicon polymer composites was revealed as a process dependent on the content of Fe and discussed in terms of heterogeneous catalysis of the shell decomposition by Fe core [Ref. 7].

Laser- and Cl atom induced chemical vapour deposition of novel polycarbosilazanes

(J. Pola, supported by Ministry of Education, Program KONTAKT, grant No. ME 684)

IR laser co-thermolysis of dimethyl selenium and 1,3-disilacyclobutane affords deposition of novel poly(selenocarbosilane) films that were revealed to react with air moisture

to produce poly(oxocarbosilanes) and volatile Se-containing compounds [Ref. 21]. IR laser gas-phase co-decomposition of alkoxysilane and alkyl borates has been found as a suitable method for synthesis of nanostructured polyborocarbosiloxanes with high content of Si-O-B bonds [Ref. 11]. MW UV laser photolysis of tetramethyldisilazane and hexamethyldisilazane in the gas phase affords chemical deposition of polycarbosilazane films that undergo hydrolysis in air. Thermal evolution of this material studied by thermal gravimetry shows this material as an efficient precursor for novel silicon carbonitrideoxide films [Ref. 20].

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 [Refs. 2, 12]. The composites show superior thermal stability.

Laser photolysis of trimethylsilylated cyclotrisilane and cyclotetrasilane

(J. Pola, supported by KONTAKT collaborative project, grant 2004-2)

ArF laser photolysis of trimethylsilylated cyclotrisilane and cyclotetrasilane in solution is an efficient route for polysilanes that are produced together with siloxanes due to interaction of transient species with traces of moisture.

New approach for the deposition of Si/Ge/C materials: Laser ablative decomposition of frozen silagermanes

(V. Dřínek, supported by ICPF)

Conventional pyrolysis and laser ablation of linear poly(germasilaethene) 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(germasilaethene) results in depletion of triple C-C bonds and crosslinking. Conventional pyrolysis of the crosslinked polymer affords polymeric material with the same Si/Ge ratio.

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

CEA Saclay DRECAM, Gif sur Yvette, France: Laser production of polyborocarbosiloxanes
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
(1 month)

Visitors

P. Papagiannakopoulos, University of Crete, Heraklion, Greece
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
F. Dumitrache, National Institute for Lasers, Plasma and Radiation Physics, Bucharest, Romania

Publications

Original papers

1. Blazevska-Gilev J., Kupčik J., Šubrt J., Vorlíček V., Galíková A., Pola J.: IR Laser-Induced Modification of Poly(vinyl acetate): Elimination of Monomer and Deposition of Polar Crosslinked Films. *Polymer* 46(21), 8973-8980 (2005).
2. Díaz L., Santos M., Ballesteros C., Maryško M., Pola J.: IR Laser-Induced Chemical Vapor Deposition of Carbon-Coated Iron Nanoparticles Embedded in Polymer. *J. Mater. Chem.* 15(40), 4311-4317 (2005).
3. Dřínek V., Vacek K., Pola J., Yuzhakov G., Šolcová O., Naumov S.: Characterization of Deposits Produced by TEA CO₂ Pulsed Laser Ablation of Silicon Mono- and Dioxide. *J. Non-Cryst. Solids* 351(2), 116-123 (2005).
4. Dřínek V., Vacek K., Yuzhakov G., Bastl Z.: Interaction between the Silyl and Silylen Centres in the Deposits Prepared by Pulsed Laser Ablation of Silicon Monoxide and Ammonia, Methylamine and Dimethylamine. *Appl. Phys. A* 81(5), 1019-1023 (2005).
5. Durani S.M.A., Khawaja E.E., Masoudi H.M., Bastl Z., Šubrt J., Galíková A., Pola J.: IR Laser Ablative Desulfurization of Poly(1,4-phenylene sulfide). *J. Anal. Appl. Pyrolysis* 73(1), 145-149 (2005).
6. Fajgar R., Hassler K., Pola J.: Laser Powered Homogeneous Decomposition of 2,2-Diethenylhexamethyltrisilane. *J. Anal. Appl. Pyrolysis* 73(2), 284-289 (2005).
7. Galíková A., Bastl Z., Alexandrescu R., Morjan I., Pola J.: Thermal Behaviour of Polyoxocarbosilane Shells in Fe-based (Core) – Polyoxocarbosilane (Shell) Nanocomposites. *Thermochim. Acta* 439(1-2), 80-85 (2005).
8. Kupčik J., Blazevska-Gilev J., Pola J.: IR Laser-Induced Degradation of Poly(vinyl acetate): Novel Thermal Reactions in the Solid Polymers. *Macromol. Rapid Commun.* 26(5), 386-389 (2005).

9. Morita H., Semba K., Bastl Z., Šubrt J., Pola J.: N₂ Laser-Induced Formation of Copolymeric Ultrafine Particles in a Gaseous Tetraethenylgermane-Carbon Disulfide Mixture. *J. Photochem. Photobiol., A* 171(1), 21-26 (2005).
10. Ouchi A., Tsunoda T., Bastl Z., Maryško M., Vorlíček V., Boháček J., Vacek K., Pola J.: Solution Photolysis of Ferrocene into Fe-based Nanoparticles. *J. Photochem. Photobiol., A* 171(3), 255-260 (2005).
11. Pola J., Herlin-Boime N., Brus J., Bastl Z., Vacek K., Šubrt J., Vorlíček V.: IR Laser Production of Nano-Structured Polyborocarbosiloxane Powders with Si-O-B Bonds. *Solid State Sci.* 7(1), 123-131 (2005).
12. Pola J., Maryško M., Vorlíček V., Bastl Z., Galíková A., Vacek K., Alexandrescu R., Dumitrache F., Morjan I., Albu L., Prodan G.: Infrared Laser Synthesis and Properties of Magnetic Nano-Iron-Polyoxocarbosilane Composites. *Appl. Organometal. Chem* 205(19), 1015-1021 (2005).
13. Pola J., Pokorná D., Diáñez M.J., Sayagués M.J., Bastl Z., Vorlíček V.: IR Laser-Induced Synthesis of Nanostructured Germanium Telluride in the Gas Phase. *Appl. Organometal. Chem* 19(7), 854-858 (2005).
14. Tomovska R., Vorlíček V., Boháček J., Šubrt J., Pola J.: ArF Laser Photolysis of Gaseous CS₂ - (CH₃)₄Sn Mixture: Gas-Phase Reaction between Tin and Sulfur and Deposition of Nano-Sized Tin Sulfides Incorporated in Polymer Network. *New J. Chem.* 29(6), 785-788 (2005).
15. Urbanová M., Pokorná D., Ouchi A., Pola J.: Laser Powered Homogeneous Decomposition of Selenophene and Tellurophene. *J. Anal. Appl. Pyrolysis* 73(1), 101-106 (2005).
16. Blazevska-Gilev J., Kupčík 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).
17. Kupčík J., Blazevska-Gilev 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.*, submitted.
18. Morita H., Nozawa R., Bastl Z., Šubrt J., Pola J.: Photochemical Synthesis of Ultrafine Organosilicon Particles from Trimethyl(2-propynyl)oxy)silane and Carbon Disulfide. *J. Photochem. Photobiol. A*, in press.
19. 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*, in press.
20. Pola J., Galíková A., Bastl Z., Šubrt J., Vacek K., Ouchi A.: UV Laser Chemical Vapour Deposition of Nanostructured Si/C/O/N/H Precursor to Silicon Oxycarbonitride. *J. Non-Cryst. Solids*, submitted.
21. 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*, in press.

Patents

22. Ouchi A., Pola J., Bastl Z., Vacek K., Šubrt J., Boháček J.: Manufacturing Method for Carbon Materials. Pat. No. JP2004-117330. Applied: 04.04.12.

Conferences

23. Blazevska-Gilev J., Kupčík J., Vorlíček V., Galíková A., Spaseska D., Pola J.: Pulsed IR Laser Ablation of Poly(Vinyl Chloride). *Polimerni materijali i dodatci polimerima, Zbornik*, p. 35-40, Zagreb, Macedonia, 17-18 November 2005.
24. Díaz L., Santos M., Ballesteros C., Pola J.: IR Laser Induced Gas-Phase Deposition of Iron Nanoparticles Embedded in a Polymeric Matrix. *2nd Nanospain Workshop, Book of Abstracts*, p. 1, Barcelona, Spain, 14-17 March 2005.
25. Dřinec V., Fajgar R., Schneider P., Šnajdaufová H., Šolcová O.: Textural Properties of Silicon Materials Produced by Laser Action. *7th International Symposium on the Characterisation of Porous Solids COPS VII, Abstracts*, p. 50, Aix-en-Provence, France, 25-28 May 2005.

26. Kupčik J., Blaževska-Gilev J., Galíková A., Pola J.: Pulsed IR Laser Ablation of Poly(Vinyl Acetate). Polimerni materijali i dodatci polimerima, Zbornik, p. 58-63, Zagreb, Macedonia, 17-18 November 2005.
27. Tomovska R., Vorlíček V., Boháček J., Šubrt J., Pola J.: ArF Laser Photolytic Deposition of Nano-Sized Tin Sulfides Incorporated in Polymer Network. 1st South European Congress of Chemical Engineering, Abstracts, Belgrade, 25-28 September 2005.
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.

Department of Analytical Chemistry

Head: J. Schraml
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E. Macháčková, L. Soukupová, J. Sýkora
Technical staff: J. Lněničková, P. Žáček

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

The ^{29}Si - ^{13}C couplings in the Si-O-C fragment

(J. Sýkora, supported by GA CR, grant No. 203/02/D176)

The main aim of this project is to describe how various substituents affect values of $2J(^{29}\text{Si}-^{13}\text{C})$ couplings in the model compounds containing Si-O-C fragment. [Ref. 6]

NMR spectroscopy in solutions

(J. Schraml, supported by GA CR, grant No. 203/03/1566)

Three relatively independent topics are being studied in solution state: ^{29}Si – ^{13}C spin-spin coupling constants, DOSY, and LC-NMR. [Refs. 4, 6, 7, 12, 14]

Enzymatic catalysis in supercritical carbon dioxide

(Participation in the project supervised by H. Sovová, joint project with Institute of Organic Chemistry and Biochemistry AS CR 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 . [Refs. 5, 10, 13]

International co-operations

University of Ghent, Ghent, Belgium: Study of neurotoxins as food contaminants

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. Círka V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry III. Photochemistry of 4-tert-Butylphenol. *J. Photochem. Photobiol., A* 174(1), 38-44 (2005).
2. Himl M., Pojarová M., Stibor I., Sýkora J., Lhoták P.: Stereoselective Alkylation of Thiocalix[4]arenes. *Tetrahedron Lett.* 46(3), 461-464 (2005).
3. Kroutil J., Karban J.: Preparation of N-nosyl-3,4-epimines Derived from Levoglucosan by Sodium Borohydride Reduction. *Carbohydr. Res.* 340(3), 503-506 (2005).
4. Řeřicha R., Blechta V., Soukupová L., Císařová I., Podlaha J., Schraml J.: On Interpretation of a Missing Spectral Band; IR Spectra of Acidic Salts of Benzohydroxamic Acid. *Spectrochim. Acta, Part A* 61(8), 1899-1903 (2005).
5. Sajfrtová M., Sovová H., Opletal L., Bártlová M.: Near-Critical Extraction of β -Sitosterol and Scopoletin from Stinging Nettle Roots. *J. Supercrit. Fluids* 35(2), 111-118 (2005).
6. Schraml J., Blechta V., Sýkora J., Soukupová L., Cuřínová P., Proněk D., Lachman J.: Characterization of Polyphenols from Plant Materials through Their Silylation and ^{29}Si NMR Spectroscopy - Line Assignment through ^{29}Si , ^{13}C Spin-Spin Couplings. *Magn. Reson. Chem.* 43(10), 829-834 (2005).
7. Schraml J., Tkadlecová M., Pataridis S., Soukupová L., Blechta V., Roithová J., Exner O.: Ring-Substituted Benzohydroxamic Acids: ^1H , ^{13}C and ^{15}N NMR Spectra and NHOH Proton Exchange. *Magn. Reson. Chem.* 43(7), 535-542 (2005).
8. Sýkora J., Budka J., Lhoták P., Stibor I., Císařová I.: Two Structural Types of 1,3-Alternate Tetrapropoxycalix[4]arene Derivatives in the Solid State. *Org. Biomol. Chem.* 3(14), 2572-2578 (2005).
9. Šťastný V., Stibor I., Petříčková H., Sýkora J., Lhoták P.: Thiocalix[4]arene Derivatives with Proximally Bridged Lower Rim. *Tetrahedron* 61(42), 9990-9995 (2005).
10. 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.*, submitted.
11. Blajiev O., Terry H., Hubin A., Soukupová L., Geerlings P.: Adsorption of Some Benzohydroxamic Acid Derivatives on Cooper Oxide: Assignment and Interpretation of SERS Spectra. *J. Raman. Spectrosc.*, in press.
12. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus J.: Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.*, in press.
13. 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.

14. Šabata S., Blechta V., Včelák J., Hetflejš J.: Selective Synthesis of Z-1,4-Disilyl-2-butenes. J. Organomet. Chem., submitted.

Conferences

15. 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. 4th International Symposium on Separations in the BioSciences (SBS'05), Symposium Program & Abstracts, p. 76, Utrecht, Netherlands, 18-21 September 2005.
16. Bernášek P., Zarevúcka M., Sovová H., Bártlová M., Stránský K., Cvačka J.: Blackcurrant Oil Hydrolysis in SC-CO₂: Experiment and Model. 10th European Meeting on Supercritical Fluids, Book of Abstracts, p. N15, Colmar, France, 12-14 December 2005.
17. Blechta V., Sýkora J., Hetflejš J., Šabata S., Schraml J.: LC-NMR of Organosilicon Polymers with Indirect ²⁹Si NMR Detection for Polymer Identification. 14th International Symposium on Organosilicon Chemistry ISOSXIV, Program, Abstracts, and List of Participants, p. P 184, Würzburg, Germany, 31 July - 05 August 2005.
18. Cuřínová P., Budka J., Rong G., Dehaen W., Schraml J.: Selective Receptors for an Ion Pair Based on Calix[4]arene. 20th NMR Valtice, Book of Abstracts, p. 47, Valtice, Czech Republic, 04-06 April 2005.
19. Sýkora J., Blechta V., Cuřínová P., Soukupová L., Schraml J.: Small J(²⁹Si-O-13) Couplings as a ²⁹Si Chemical Shift Assignment Tool. 14th International Symposium on Organosilicon Chemistry ISOSXIV, Program, Abstracts, and List of Participants, p. P 185, Würzburg, Germany, 31 July - 05 August 2005.
20. Sýkora J., Blechta V., Cuřínová P., Soukupová L., Schraml J.: Small Long-Range J(²⁹Si-O-13C) Couplings as an ²⁹Si Chemical Shift Assignment Tool. 20th NMR Valtice, Book of Abstracts, p. 11, Valtice, Czech Republic, 04-06 April 2005.

Miscellaneous

International Advisory Board of ICPF

Prof. V. Bálež, Slovak Technical University, Bratislava, Slovakia
Prof. L. S. Fan, Ohio State University, Columbus, USA
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Memberships in Editorial Boards

J. Drahoš: "International Journal of Multiphase Flow"
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I. Wichterle: "Chemical Engineering and Technology"
I. Wichterle: "Fluid Phase Equilibria"
V. Ždímal: "Aerosol and Air Quality Research"

Hála Lectures

First (1999)	Arnošt REISER (Polytechnic University, Brooklyn, New York, USA) "Remembering Eduard Hála"
Second (2000)	Gerhart EIGENBERGER (Universität Stuttgart, Stuttgart, Germany) "Membrane Fuel Cell Systems: A Challenge for Chemical Engineers"
Third (2001)	David AVNIR (Hebrew University, Jerusalem, Israel)

- Fourth (2002) "The Measurement of Symmetry and Chirality: Concept and Applications across Chemistry"
William R. SMITH (Guelph University, Guelph, Canada)
"Macroscopic- and Microscopic-Level Thermodynamics: Partners in Chemical Engineering Progress"
- Fifth (2003) Jakob de Swaan Arons (Delft University of Technology, the Netherlands)
"Economy, Ecology and Thermodynamics"
- Sixth (2004) Vladimír Hlaváček, (State University of New York, Buffalo, USA)
"Reactivity, Stored Energy, and Dislocations in Solid Reacting Systems"
- Seventh (2005) Jean-Claude Charpentier (President of EFCE, CNRS–INPL, Nancy, France)
"In the Frame Globalization and Sustainability: Evolution of Chemical and Process Engineering – Progression from Commodities to New Specialties and Active Material Chemistry"