

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 2002

Address Institute of Chemical Process Fundamentals
Academy of Sciences of the Czech Republic
Rozvojová 135
165 02 Prague 6 - Suchbát
Czech Republic

Telephone +420 220390 111
+420 296780 111

Telefax +420 22092 0661

E-mail icecas@icpf.cas.cz

Internet <http://www.icpf.cas.cz>

© 2003, Institute of Chemical Process Fundamentals ASCR, Prague
Edited by J. Linek

ISBN 80-86186-08-3

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 engineering, physical chemistry, industrial chemistry, and biotechnology.

MANAGEMENT

| | |
|---|-------------|
| Director | Jiří Drahoš |
| Deputy Director (Research) | Jan Čermák |
| 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 12)
Department of Catalysis and Reaction Engineering (page 20)
Department of Multiphase Reactors (page 27)
Department of Biotechnology and Environmental Processes (page 33)
Department of Reaction Engineering in Gas Phase (page 39)
Department of Analytical Chemistry (page 57)

STAFF
(31 December 2002)

| Category | Number of Employees |
|----------------|---------------------|
| Research | 111 |
| Technical | 24 |
| Administrative | 16 |
| Services | 14 |

BUDGET 2002
(in million Kč; 33 Kč = 1 US\$, approx.)

| | |
|--|----|
| Institutional support from National Budget | 49 |
| Research funds from Grant Agencies | 40 |
| Contracts with industry | 3 |

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 Diffusion and Separation Processes

Head: V. Jiříčný
Deputy: A. Heyberger
Research staff: L. Hanková, P. Izák, K. Jeřábek, J. Procházka, Z. Prokop, H. Sovová,
P. Uchytíl, J. Voborská, E. Volaufová
Part time: V. Staněk, H. Vychodilová
Technical staff: L. Holub, A. Kadlecová, D. Karfík, M. Koptová, R. Petříčkovič, D. Vlček
PhD students: K. Fialová, J. Ondráček, M. Sajfrtová, P. Svoboda, P. Veverka

Fields of research

- Gas capillary condensation in small pores of inorganic membranes and its influence on membrane separation properties
- Relation between the morphology and application properties of polymer catalysts and adsorbents
- Hydrodynamic study of dynamic behaviour of two-phase counter-current gas-liquid flow in packed bed column around flooding
- Reactive liquid-liquid extraction of inorganic acids with amines and effect of solvating diluents. Liquid extraction of drinking and surface waters for the determination of toxic pollutants
- Supercritical fluid extraction of natural products; enzymatic reactions in supercritical CO₂; solubilities of liquids and solids in dense CO₂ with entrainer

Applied research

- Extraction aided determination of organic pollutants in waters
- Refining of plant extracts
- Supercritical fluid extraction of biologically active substances from plants
- Preparation of corundum support for ceramic membranes
- Analysis of function of the catalytic reactor for bisphenol A synthesis and research of the catalytic deactivation
- Electrowinning of metals using three-dimensional electrodes

Research projects

Relations between morphology and activity of ion exchanger catalysts in non-aqueous environment

(K. Jeřábek, supported by GA CR, grant No. 104/02/1104)

Relations are investigated between morphology and activity of ion exchange resin catalysts for industrially important reactions. Information on swollen state morphology of ion exchanger catalysts obtained by inverse steric exclusion chromatography (ISEC) has been used for elucidation of mechanisms by which polymer structure controls activity of ion exchanger catalysts of industrially important reactions in non-aqueous environment. [Refs. 4, 32]

Fundamental research of appearance of pressure and liquid holdup overshoot as a new phenomenon in hydrodynamic behavior of counter-current packed beds

(V. Staněk, supported by GA ASCR, grant No. A4072004)

The pressure and liquid hold up overshoot following sudden increase of gas or liquid flow have been experimentally studied in counter-current packed bed column around flooding point. A mathematical model has been developed to describe the results. [Refs. 34, 42, 47]

Effect of diluent type and composition on extraction of mineral acids with tertiary amines

(A. Heyberger, GA CR, grant No. 104/02/1108)

Equilibria of sulfuric acid extraction from aqueous solutions with trialkylamine in octanol/kerosene and xylene/kerosene mixtures were measured and correlated with a mathematical model. The effects of amine content and diluent composition on extraction equilibrium were investigated. [Refs. 17, 46]

Liquid extraction of tall oil

(A. Heyberger, joint project with Institute of Landscape Ecology AS CR and School of Science and Technology, Meiji University, Japan, supported by Ministry of Education, grant No. ME 608)

Main goal of the project is to find an effective organic solvent, or solvent mixture, for extraction of the crude tall oil and for separation of the fraction of fatty and resin acids with high yields.

Supercritical fluid extraction of plant metabolites usable in the treatment and prevention of the diseases of heart and vessels

(H. Sovová, joint project with Faculty of Pharmacy CU, supported by GA CR, grant No. 203/01/0550)

Biologically active substances were extracted from leaves and roots of stinging nettle (*Urtica dioica* L.) with CO₂ modified by ethanol. The yields of chlorophylls, carotenoids, β -sitosterol, scopoletin and homovanillyl alcohol were determined using HPLC. The research was concentrated on the following topics: chlorophyll degradation to pheophytin, effect of operating conditions on the extraction rate of low-polar and polar solutes, solute-matrix interaction and mutual interaction of extracted substances, and mathematical model of the extraction process. [Refs. 18, 19, 35, 37, 40, 41]

A potential of nanofiltration layers for membrane separation of light aliphatic hydrocarbons

(P. Uchytíl, joint project with J. Heyrovsky Institute of Physical Chemistry ASCR, Institute of Physics ASCR and Institute of Chemical Technology, Prague, supported by GA CR, grant No. 104/01/0945)

New sorption and permeation apparatus for the study of surface phenomena during gas transport in Vycor glass pores has been developed and manufactured. The influence of these

phenomena on the separation efficiency in Vycor membrane has been experimentally verified. [Refs. 22, 43, 44]

International co-operations

Otto von Guericke University of Magdeburg, Magdeburg, Germany: Determination of porous structure of ceramic membranes
Hiroshima University, Hiroshima, Japan: Pervaporation on ceramic membranes
Meiji University, School of Science and Technology, Tama-ku, Japan: Extraction of tall oil.
University of Padua, Padua, University of L'Aquila, L'Aquila, Italy: Molecular accessibility of microporous matrixes
Weizmann Institute of Science, Rehovot, Israel: Novel selective sorbents
Technical University, Bratislava, Slovakia: Polymer supported catalysts
University of Strathclyde, Strathclyde, Glasgow, Great Britain: Morphology of functional polymers
University of Stellenbosh, Stellenbosh, Republic of South Africa: Modelling of back mixing in vibrating-plate extractor
University of Linz, Linz, Austria: Determination of organic pollutants in water
Institute of Chemical Engineering, Sofia, Bulgaria: Separation of heavy metals from aqueous solutions using amine extractants; high-pressure phase equilibria
University of Skopje, Skopje, Macedonia: Extraction of hydroxycarboxylic acids, supercritical fluid extraction of natural products
CSIR of Pretoria and Johannesburg, Johannesburg, Republic of South Africa: Liquid-Liquid extraction process
University of California, Berkeley, USA: Research and development of three-dimensional electrodes for metal electrowinning

Visits abroad

A. Heyberger: University of Durban, AECI, CSIR, Johannesburg, Republic of South Africa (7 weeks)
V. Jiříčný: University of California, Berkeley, USA (4 weeks)

Visitors

S. Aleksovski, University of Skopje, Macedonia
S. Boyadzhieva, Institute of Chemical Engineering, Sofia, Bulgaria
B. Corain, University of Padua, Italy
A.A. Galushko, Institute of Chemical Engineering, Sofia, Bulgaria
K. Kruusement, Tallinn Technical University, Estonia
W. Kujawski, Copernicus University, Torun, Poland
R.P. Stateva, Institute of Chemical Engineering, Sofia, Bulgaria

Teaching

K. Jeřábek: ICT, postgraduate course "Preparation of the heterogeneous catalysts"

Publications

Original papers

1. Bártlová M., Opletal L., Chobot V., Sovová H.: Liquid Chromatographic Analysis of Supercritical Carbon Dioxide Extracts of *Schizandra chinensis*. *J. Chromatogr.*, B 770(1-2), 283-289 (2002).
2. Biffis A., Ricoveri R., Campestrini S., Králik M., Jeřábek K., Corain B.: Highly Chemoselective Hydrogenation of 2-Ethylanthraquinone to 2-Ethylanthrahydroquinone Catalyzed by Palladium Metal Dispersed inside Highly Lipophilic Functional Resins. *Chem. Eur. J.* 8(13), 2962-2967 (2002).
3. Hrma P., Izák P., Vienna J.D., Thomas M.-L., Irwin G.M.: Partial Molar Liquidus Temperatures of Multivalent Elements in Multicomponent Borosilicate Glass. *Phys. Chem. Glasses* 43(2), 119-127 (2002).
4. Jeřábek K., Hanková L., Prokop Z., Lundquist E.G.: Relations Between Morphology and Catalytic Activity of Ion Exchanger Catalysts for Synthesis of Bisphenol A. *Appl. Catal., A* 232(1-2), 181-188 (2002).
5. Jiříčný V., Roy A., Evans J.W.: Copper Electrowinning using Spouted-Bed Electrodes: Part I. Experiments with Oxygen Evolution or Matte Oxidation at the Anode. *Metall. Mater. Trans. B* 33(5), 669-676 (2002).
6. Jiříčný V., Roy A., Evans J.W.: Copper Electrowinning using Spouted-Bed Electrodes: Part II. Copper Electrowinning with Ferrous Ion Oxidation as the Anodic Reaction. *Metall. Mater. Trans. B* 33(5), 677-683 (2002).
7. Uchytíl P., Petříčkovič R.: Vapor Permeation and Pervaporation of Propan-1-ol and Propan-2-ol in Polyethylene Membrane. *J. Membr. Sci.* 209, 67-79 (2002).
8. Warshawsky A., Strikovsky A.G., Vilensky M.Y., Jeřábek K.: Interphase Mobility and Migration of Hydrophobic Organic Metal Extractant Molecules in Solvent Impregnated Resins. *Sep. Sci. Technol.* 37(11), 2607-2622 (2002).
9. Warshawsky A., Strikovsky A.G., Fernandez F.M., Jeřábek K.: Synthesis of Novel Chelating Resins Containing Dithiophosphoric Functionality and Comparison to Analogous Solvent-Impregnated Resins (SIR's). *Sep. Sci. Technol.* 37(4), 823-846 (2002).
10. Artuso F., D'Archivio A.A., Jeřábek K., Corain B.: Polymer Framework as Templates for Generating Size-Controlled Metal Nanoclusters. *Synthetic Aspects. Adv. Mater.*, submitted.
11. Bombi G., Palma G., Lora S., Zancato M., D'Archivio A.A., Jeřábek K., Corain B.: Generating Palladium Nanoclusters Inside Very Lipophilic Gel-Type Functional Resins. Preliminary Catalytic Test in the Hydrogenation of 2-Ethyl-Anthraquinone to 2-Ethyl-anthrahydroquinone. *J. Mol. Catal. A: Chem.*, submitted.
12. Durie S., Jeřábek K., Mason C., Sherrington D.C.: One-pot Synthesis of Branched Poly(Styrene-Divinylbenzene) Suspension Polymerised Resins. *Macromolecules*, submitted.

13. Izák P., Bartovská L., Friess K., Šípek M., Uchytíl P.: Comparison of Various Models for Transport of Binary Mixtures through Dense Polymer Membrane. *J. Polym.*, in press.
14. Izák P., Bartovská L., Friess K., Šípek M., Uchytíl P.: Description of Binary Liquid Mixtures Transport through Non-porous Membrane by Modified Maxwell-Stefan Equations. *J. Membr. Sci.*, in press.
15. Pavlů J., Kudová J., Zikánová A., Kočířik M., Uchytíl P., Šolcová O., Roček J., Fíla V., Bernauer B., Krystl V., Hrabánek P.: Keramické porézní elementy pro filtraci plynů a příbuzné aplikace. (Czech) Ceramic Porous Elements for Gas Separation and Related Applications. *Chem. Listy*, in press.
16. Poposka F.A., Procházka J., Nikolovski K., Tomovska R.: Extraction of Tartaric Acid from Aqueous Solutions with Tri-iso-octylamine (HOSTAREX A 324). Simulation on the Process in a Reciprocating-Plate Extraction Column. *Bull. Chem. Technol. Macedonia*, submitted.
17. Procházka J., Heyberger A., Volaufová E.: Sulfuric Acid Extraction with Tertiary Amines - Effect of Xylene and n-Octanol as Diluents. *Ind. Eng. Chem. Res.*, in press.
18. Sovová H.: Mathematical Model for Supercritical Fluid Extraction of Natural Products and for Extraction Curves Evaluation. *J. Supercrit. Fluids*, in press.
19. Sovová H., Sajfrtová M., Bártlová M., Opletal L.: Near-critical Extraction of Pigments and Oleoresin from Stinging Nettle Leaves. *J. Supercrit. Fluids*, submitted.
20. Sovová H., Zarevúcka M.: Lipase-catalyzed Hydrolysis of Blackcurrant Oil in Supercritical Carbon Dioxide. *Chem. Eng. Sci.*, in press.
21. Turacchio M., Di Nino G., D'Archivio A.A., Jeřábek K., Lora S., Antonini G., Corain B.: Nanostructure and Molecular Accessibility of Gel-Type Resins for Supported Catalysis. Part I. Polyhydroxyethylmethacrylate-Hydroxypropylmethacrylate-Trimethylolpropane Trimethacrylate. *React. Func. Polym.*, submitted.
22. Uchytíl P., Petříčkovič R., Thomas S., Siedel-Morgenstern A.: Influence of Capillary Condensation Effects on Mass Transport through Porous Membranes. *J. Sep. Pur. Technol.*, in press.
23. Veverka P., Jeřábek K.: Influence of Hypercrosslinking on Adsorption and Absorption on or in Styrenic Polymers. *React. Func. Polym.*, submitted.

Theses

24. Izák P.: Pervaporation of Liquid Organic Mixtures. PhD Thesis, Institute of Chemical Technology, Prague 2002.

Conferences

25. Evans J.W., Jiříčný V.: Spouted Bed Electrodes: a Review. 52e Congrès canadien de génie chimique, Programme final, p. 288, Vancouver, Canada, 20-23 October 2002.
26. Friess K., Šípek M., Hynek V., Bohatá K., Izák P., Sysel P.: Permeability of Polymer Membranes for Organic Vapors. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 268, Prague, Czech Republic, 25-29 August 2002.
27. Friess K., Šípek M., Hynek V., Izák P., Sysel P.: Sorption of Organic Vapors in Polymer Membranes. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 237, Prague, Czech Republic, 25-29 August 2002.
28. Friess K., Šípek M., Hynek V., Izák P., Sysel P.: Study of Sorption of Organic Vapors in Polymer Membranes. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 192, Tatranské Matliare, Slovakia, 27-31 May 2002.

29. García A., Heyberger A., Procházka J., Canete R., Vinals M.: Natural Wax Refining by Liquid/Liquid Extraction. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 220, Prague, Czech Republic, 25-29 August 2002.
30. Izák P., Bartovská L., Šípek M., Uchytíl P., Friess K., Machková J., Habrdová K.: Separation Properties of a Polyethylene Membrane and Model Calculations. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 236, Prague, Czech Republic, 25-29 August 2002.
31. Izák P., Bartovská L., Šípek M., Friess K., Uchytíl P.: Description of Transport Properties of Binary Liquid Mixtures through Polyethylene Membrane by Modified Maxwell-Stefan Model. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 208, Tatranské Matliare, Slovakia, 27-31 May 2002.
32. Jeřábek K., Hanková L., Prokop Z., Lindquist E.G.: Relations between Morphology and Catalytic Activity of Ion Exchanger Catalysts for Synthesis of Bisphenol A. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 99, Tatranské Matliare, Slovakia, 27-31 May 2002.
33. Jiříčný V., Evans J.W., Roy A.: Spouted Beds for the Electrodeposition of Copper. 52e Congrès canadien de génie chimique, Programme final, p. 289, Vancouver, Canada, 20-23 October 2002.
34. Ondráček J., Jiříčný V., Staněk V.: Operation of a Bubble Bed in Series with a Trickle Bed. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 71, Prague, Czech Republic, 25-29 August 2002.
35. Opletal L., Sovová H., Bártlová M.: Metoda extrakce superkritickými tekutinami (SFE) v produkci léčivých látek a ve farmaceutické analýze. (Czech) Supercritical Fluid Extraction (SFE) in Production of Medical Substances and in Pharmaceutical Analysis. XXXI. konferencia Syntéza a analýza liečiv, Sborník abstraktů, p. 5, Bratislava, Slovakia, 11-13 September 2002.
36. Procházka J., Heyberger A., Volaufová E.: Extraction of Mo(VI) and W(VI) with Trialkylamine. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 157, Prague, Czech Republic, 25-29 August 2002.
37. Sajfírtová M., Sovová H., Bártlová M., Opletal L.: Supercritical Fluid Extraction and Characterisation of *Urtica Dioica* L. Leaves Pigments. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 279, Prague, Czech Republic, 25-29 August 2002.
38. Šípek M., Friess K., Hýnek V., Bohatá K., Izák P., Sysel P.: Permeability of Polyethylene Membranes for Organic Vapors and Their Mixtures. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 191, Tatranské Matliare, Slovakia, 27-31 May 2002.
39. Šolcová O., Uchytíl P., Schneider P.: Textural Properties of Porous Solids from Liquid Expulsion Permporometry. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 343, Prague, Czech Republic, 25-29 August 2002.
40. Sovová H.: Interpretation of Extraction Curves Obtained by Supercritical Fluid Extraction from Plant Materials. 4th International Symposium on High Pressure Technology and Chemical Engineering, Volume 2, p. 693-698, Venice, Italy, 22-25 September 2002.
41. Sovová H.: Evaluation of Extraction Curves Obtained by Supercritical Fluid Extraction from Plant Materials. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 150, Prague, Czech Republic, 25-29 August 2002.

42. Svoboda P., Staněk V., Jiříčný V.: The Behavior of a Counter-Current Packed Bed Column Undergoing Flooding. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 72, Prague, Czech Republic, 25-29 August 2002.
43. Uchytíl P., Petříčkovič R.: Gas Separation on Vycor Glass. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 82, Tatranské Matliare, Slovakia, 27-31 May 2002.
44. Uchytíl P., Petříčkovič R., Thomas S., Seidel-Morgenstern A.: Influence of Capillary Condensation Effects on Mass Transport through Porous Membranes. 7th International Conference on Inorganic Membranes, Program and Book of Abstracts, p. 16-17, Dalian, China, 23-26 June 2002.
45. Veverka P., Jeřábek K.: Influence of Hypercrosslinking on Absorption and Adsorption in/on S-DVB Polymers. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 359, Prague, Czech Republic, 25-29 August 2002.
46. Volaufová E., Heyberger A., Procházka J.: Extraction of Sulfuric Acid with Tertiary Amines in Mixtures of Xylene with Paraffinic Diluent. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 163, Tatranské Matliare, Slovakia, 27-31 May 2002.
47. Vychodilová H., Staněk V., Akramov T., Jiříčný V.: Dynamics of Absorption in Co-Current Packed Column under Periodically Variable Conditions. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 202, Prague, Czech Republic, 25-29 August 2002.

E. Hála Laboratory of Thermodynamics

Head: I. Wichterle
Deputy: K. Aim
Research staff: J. Kolafa, J. Linek, M. Lísal, L. Morávková, I. Nezbeda, J. Pavlíček,
M. Předota, J. Slovák, Z. Wagner
D. Constantinescu (visiting)
Technical staff: S. Bernatová, Š. Psutka
PhD students: A. Babič, L. Vlček

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
- Determination of pressure–volume–temperature behaviour of liquids
- Thermodynamic modelling and processing of thermodynamic data
- Development of equations of state based on molecular theory
- Molecular simulations on model fluids and fluid mixtures
- Application of statistical–mechanical models to real fluids
- Molecular modelling of solubility of liquids
- Theory of polar compounds
- Study of hydrophobic interactions
- General phase behaviour of binary mixtures – global phase diagrams

Applied research

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

Research projects

Description of thermodynamic properties of fluids at superambient conditions by the methods of applied statistical mechanics

(K. Aim, joint project with CU, supported by GA CR, grant No. 203/00/0600)

Determinations of excess volumes for systems of binary combinations of the type heptane or octane plus linear 1-chlorohydrocarbon (C_4 to C_6) at temperatures up to 330 K and pressures up to 400 bar have been completed. Second-order perturbation theory for fluids constituted of anisotropic dipolar molecules has been successfully applied to a series of linear chloroalkanes and to selected binary systems of the type linear alkane + linear chloroalkane. [Refs. 9–13, 23–25, 41, 49, 50, 53, 54, 58]

From simple models towards molecular theory of associated liquids: Theory and application

(I. Nezbeda, supported by GA ASCR, grant No. A4072908)

Computer simulations examining in detail the effect of the range of intermolecular interactions on the properties of associating fluids have been completed. Further investigations aimed at application of the basic finding, namely that the long-range forces affect the properties of fluids only marginally. A simple model of water has been thoroughly investigated and used to study the nature of hydrophobicity, hydrogen bonding, and adsorption. A complex model of real water has also been tested. [Refs. 4–7, 15, 18, 32]

High pressure phase equilibria and supercritical extraction

(I. Wichterle, supported by GA ASCR, grant No. A4072102)

Modelling of high pressure solubilities using equation of state in mixtures of alternative fuels. New model was elaborated for supercritical extraction from plants which encounters equilibrium concentration of both free and bound in matrix compound. Kinetics and equilibria have been investigated in systems containing natural raw material. High pressure phase equilibrium has been determined in the menthol + CO₂ system. The comprehensive review on solubility of solids and liquids in supercritical fluids has been published. [Refs. 34, 37, 38, 68, 69; see also Department of Diffusion and Separation Processes, Refs. 16, 35, 36]

Statistical–thermodynamic study of model colloid systems

(I. Nezbeda, supported by GA CR, grant No. 203/01/0464)

In addition to attempts to develop an equation of state for a simple model of colloid systems, mixture of hard spheres, a possibility to find a general theoretically-based expression for the pair correlation function for the same system has been explored. During the year the focus has shifted from hard sphere models to models of colloids in an aqueous environment. An approximation for future theoretical studies has been intensively tested by means of computer simulations. [Ref. 32]

Pressure–volume–temperature behaviour of liquids and liquid mixtures significant for solving the environmental problems

(J. Linek, supported by GA CR, grant No. 203/02/1098)

The project is focused on the experimental determination of P-V-T properties of pure liquids and liquid mixtures at normal and elevated temperatures and pressures (up to 330 K and 40 MPa). The apparatus used is based on the vibrating-tube densimeter (A. Paar model 58 + DMA 512P) equipped with a high-pressure line. During the first year, the apparatus was tested and three systems composed of benzene and C₃-alkylbenzenes were measured. [Refs. 21, 24, 26, 27]

Molecular model of aqueous solutions of electrolytes and its application

(I. Nezbeda, supported by GA CR, grant No. 203/02/0764)

Phenomena of structure breaking and structure enhancement in dilute solutions of aqueous electrolytes have been studied by means of a simple theoretical model, which accounts explicitly for the molecular nature of the solvent (water). The focus of the research has gradually moved from infinite dilution to solutions of finite concentration and extensive computations of the potential of mean forces have begun. [Ref. 28]

Molecular modeling of supercritical carbon dioxide–surfactant–solute systems

(M. Lísal, supported by GA CR, grant No. 203/02/0805)

We have used lattice Monte Carlo simulations and multiple equilibrium macroscopic model to study the formation of micelles and micellar solubility in supercritical solvents. We have focused on influence of solvent densities and structure of surfactants on the formation of the micelles. We have further examined various models of supercritical carbon dioxide and water in order to improve lattice models for the solvent and solute. [Refs. 2, 5–7, 17, 19, 22, 45, 51, 52, 63, 64]

Molecular thermodynamics of polar and associating fluid mixtures

(Co-researchers: J. Fischer (Institute of Environmental and Energy Engineering, University of Agricultural Sciences, Vienna) and I. Nezbeda; supported by Ministry of Education: AKTION – The Czech–Austrian co-operation program 1999–2002)

Based on results of new extensive molecular simulations for the two-center Lennard–Jones model fluid, the van der Waals-type equation of state for this class of model fluids has been revised and its validity thereby extended to the parametric region of large molecular elongations. [Refs. 22, 39]

Research Centre: Behaviour of multiphase systems under superambient conditions

(J. Drahoš, I. Wichterle, supported by EU 5th RTD NAS2 72074)

This interdisciplinary Research Centre (BEMUSAC) integrates physical chemists and chemical engineers to study and develop new processes based on gas-liquid-solid contacting. It has been established in view of significant reorientation and transformation of the R&D potential towards the advanced fields of multiphase systems under extreme conditions, namely to thermodynamic systems at high pressures and temperatures, to bubble processes in metallurgy and to hydrodynamics of rheologically complex systems.

International co-operations

DICAMP, University of Trieste, Trieste, Italy: Phase equilibria for supercritical fluid technology

University of Guelph, Guelph, Canada: Molecular based modelling of systems with phase and chemical equilibria; Solubility of organic compounds

Sonderforschungsbereich, University of Leipzig, Leipzig, Germany: Fluids in confined geometries

University of Tennessee, Knoxville, TN, USA: Simulation of complex fluid systems

ITODYS, University of Paris VII, Paris, France: Vapour–liquid equilibrium bibliographic database; Phase equilibria in selected systems

Institute of Physical Chemistry, Romanian Academy, Bucuresti, Romania: Phase equilibria in fluid systems

University of Agricultural Sciences, Vienna, Austria: Molecular thermodynamics of polar and associating fluid mixtures

Visits abroad

M. Lísal: University of Guelph, Guelph, Canada (1 month)

M. Předota: University of Tennessee, Knoxville TN, USA (4 months)

J. Slovák: University of Okayama, Japan (12 months)

Visitors

A. Ben-Naim, Hebrew University, Jerusalem, Israel (2 months)

Teaching

M. Lísal: J. E. Purkyně University, course "Parallel programming", "Numerical mathematics"

I. Nezbeda: J. E. Purkyně University, course "Molecular theory of matter"

I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"

I. Nezbeda, M. Předota: CU, course "Introduction to computer simulations in many particle systems"

Publications

Original papers

1. Čapla L., Buryan P., Jedelský J., Rottner M., Linek J.: Isothermal P-V-T Measurements on Gas Hydrocarbon Mixtures Using a Vibrating Tube Apparatus. *J. Chem. Thermodyn.* 34(5), 657-667 (2002).
2. Colina C.M., Lísal M., Siperstein F.R., Gubbins K.E.: Accurate CO₂ Joule–Thomson Inversion Curve by Molecular Simulations. *Fluid Phase Equilib.* 202(2), 253-262 (2002).
3. Constantinescu D., Wichterle I.: Isothermal Vapour–Liquid Equilibria and Excess Molar Volumes in the Binary Ethanol + Methyl Propanoate or Methyl Butanoate Systems. *Fluid Phase Equilib.* 203(1-2), 71-82 (2002).
4. Kettler M., Nezbeda I., Chialvo A.A., Cummings P.T.: Effect of the Range of Interactions on the Properties of Fluids. *Phase Equilibria in Pure Carbon Dioxide, Acetone, Methanol, and Water.* *J. Phys. Chem. B* 106(30), 7537-7546 (2002).
5. Lísal M., Hall C.K., Gubbins K.E., Panagiotopoulos A.Z.: Micellar Behavior in Supercritical Solvent-Surfactant Systems from Lattice Monte Carlo Simulations. *Fluid Phase Equilib.* 194-197, 233-247 (2002).
6. Lísal M., Hall C.K., Gubbins K.E., Panagiotopoulos A.Z.: Self-Assembly of Surfactants in a Supercritical Solvent from Lattice Monte Carlo Simulations. *J. Chem. Phys.* 116(3), 1171-1184 (2002).
7. Lísal M., Kolafa J., Nezbeda I.: An Examination of the Five-Site Potential (TIP5P) for Water. *J. Chem. Phys.* 117(9), 8892-8897 (2002).
8. Lísal M., Smith W.R., Bureš M., Vacek V., Navrátil J.: REMC Computer Simulation of the Thermodynamic Properties of Argon and Air Plasmas. *Mol. Phys.* 100(15), 2487-2497 (2002).
9. Morávková L., Aim K., Linek J.: Excess Molar Volumes of (Heptane + 1-Chloropentane) at Elevated Temperatures and High Pressures. *J. Chem. Thermodyn.* 34(9), 1377-1386 (2002).
10. Morávková L., Linek J.: Excess Molar Volumes of the Octane-1-Chlorobutane System at High Pressures and Elevated Temperatures. *Chem. Pap.* 56(6), 374-377 (2002).

11. Morávková L., Linek J.: Excess Molar Volumes of (Heptane + 1-Chlorobutane) at Elevated Temperatures and High Pressures. *J. Chem. Thermodyn.* 34(9), 1397-1405 (2002).
12. Morávková L., Linek J.: Temperature Dependence of Excess Molar Volumes of (Octane + 1-Chloroalkane). *J. Chem. Thermodyn.* 34(9), 1407-1415 (2002).
13. Morávková L., Linek J.: Temperature Dependence of Excess Molar Volumes of (Heptane + 1-Chloroalkane). *J. Chem. Thermodyn.* 34(9), 1387-1395 (2002).
14. Předota M., Cummings P.T., Chialvo A.A.: Pair Approximation for Polarization Interaction and Adiabatic Nuclear and Electronic Sampling Method for Fluids with Dipole Polarizability. *Mol. Phys.* 100(16), 2703-2717 (2002).
15. Předota M., Nezbeda I., Cummings P.T.: Hydrophobic Hydration at the Level of Primitive Models. II. Large Solutes and Water Restructuring. *Mol. Phys.* 100(14), 2189-2200 (2002).
16. Rivera J.L., Předota M., Chialvo A.A., Cummings P.T.: Vapor-Liquid Equilibrium Simulations of the SCPDP Model of Water. *Chem. Phys. Lett.* 357(3-4), 189-194 (2002).
17. Smith W., Lísal M.: Direct Monte Carlo Simulation Methods for Nonreacting and Reacting Systems at Fixed Total Internal Energy or Enthalpy. *Phys. Rev. E* 66(1), 111041-111043 (2002).
18. Vlček L., Nezbeda I.: Size and Shape Dependence of Hydrophobic Hydration at the Level of Primitive Models. *Phys. Chem. Chem. Phys.* 4(15), 3704-3711 (2002).
19. Colina C.M., Olivera-Fuentes C.G., Siperstein F.R., Lísal M., Gubbins K.E.: Thermal Properties of Supercritical Carbon Dioxide by Monte Carlo Simulations. *Mol. Simul.*, in press.
20. Dragoescu D., Teodorescu M., Barhala A., Wichterle I.: DISQUAC Characterization of the Carbonyl-Chlorine Interactions in Binary Mixtures of Linear Ketone with Chloroalkane. *Collect. Czech. Chem. Commun.*, submitted.
21. Linek J.: Letter to the Editor: About "Studies of viscosity and excess molar volume of binary mixtures of propane-1,2 diol with water at various temperature". *Fluid Phase Equilib.*, submitted.
22. Lísal M., Aim K., Mecke M., Fischer J.: The Equation of State for Two-Center Lennard-Jones Fluids Revised. *Int. J. Thermophys.*, submitted.
23. Morávková L., Linek J.: Excess Molar Volumes of (Octane + 1-Chlorobutane) between Temperatures 298.15 K and 328.15 K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.*, in press.
24. Morávková L., Linek J.: Excess Molar Volumes of (Octane + 1-Chloropentane) between Temperatures 298.15 K and 328.15 K and at pressures up to 40 MPa. *J. Chem. Thermodyn.*, submitted.
25. Morávková L., Linek J.: Excess Molar Volumes of (Octane + 1-Chlorohexane) between Temperatures 298.15 K and 328.15 K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.*, in press.
26. Morávková L., Linek J.: Excess Molar Volumes of (Benzene + Isopropylbenzene, or 1,3,5-Trimethylbenzene, or 1,2,4-Trimethylbenzene) at Temperatures between 298.15 K and 328.15 K. *J. Chem. Thermodyn.*, submitted.
27. Morávková L., Wagner Z., Linek J.: (P, V, T, x) Measurements of the Benzene + 1,3,5-Trimethylbenzene System at Temperatures from 298.15 K to 328.15 K and at Pressures up to 40 MPa. *Fluid Phase Equilib.*, submitted.
28. Nezbeda I.: Modeling of Aqueous Electrolytes at the Molecular Level: On the Origin of the Structure Breaking and Structure Enhancement Phenomena. *J. Mol. Liq.*, in press.
29. Nezbeda I.: Towards a Unified View of Fluids. *Mol. Phys.*, in press.

30. Pavlíček J., Aim K., Boublík T.: Fluids of the Kihara Molecules. II. Binary Mixtures of n-Alkanes. *J. Phys. Chem.*, in press.
31. Pavlíček J., Aim K., Boublík T.: Fluids of Polar and Polarizable Kihara Molecules. I. Pure Linear Chloroalkanes. *J. Phys. Chem.*, submitted.
32. Předota M., Ben-Naim A., Nezbeda I.: On Independence of the Solvation of Interaction Sites of a Water Molecule. *J. Chem. Phys.*, submitted.
33. Slovák J., Nezbeda I.: On Accuracy of Wertheim's Thermodynamic Perturbation Theory for Primitive Models of Water. *Mol. Phys.*, in press.
34. Teodorescu M., Wichterle I.: Modeling of the Nitrogen and Carbon Dioxide Solubility in Alternative Fuels at High Pressures using Soave-Redlich-Kwong Equation of State. *Chem. Eng. Technol.*, submitted.
35. Vlček L., Nezbeda I.: A Primitive Model of Methanol. *Mol. Phys.*, submitted.

Books and monographs

36. Wichterle I., Linek J., Wagner Z., Kehiaian H.V.: Vapor-Liquid Equilibrium in Mixtures and Solutions. Bibliographic Database. ELDATA, Paris, in press.

Chapters in books

37. Aim K., Fermeglia M.: Solubility of Solids and Liquids in Supercritical Fluids. In: *The Experimental Determination of Solubilities*. (Hefter, G. T. - Tomkins, R. P. T., Ed.), pp. 491-553, John Wiley&Sons 2002.

Conferences

38. Aim K., Babič A.: A New Apparatus for High-Pressure Fluid Phase Equilibrium Measurements at Elevated Temperatures. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 301, Prague, Czech Republic, 25-29 August 2002.
39. Aim K., Fischer J., Lísal M., Mecke M.: The Equation of State for Dipolar Two-Centre Lennard-Jones Fluid Revised for Extended Range of Elongations. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
40. Aim K., Lísal M.: Calculation of Binary Vapour-Liquid Equilibria by the Reaction Gibbs Ensemble Monte Carlo Simulation Method. 19th European Conference on Applied Thermodynamics ESAT 2002, Santorini, Greece, 06-10 September 2002.
41. Aim K., Lísal M., Pavlíček J.: Molecular-Based Modelling of Equilibrium Fluid Properties at Superambient Conditions. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 100, Prague, Czech Republic, 25-29 August 2002.
42. Aim K., Wichterle I.: Vapour-Liquid and Chemical Reaction Equilibria in Three Quaternary Esterification Systems. 19th European Conference on Applied Thermodynamics ESAT 2002, Santorini, Greece, 06-10 September 2002.
43. Chialvo A.A., Nezbeda I., Cummings P.T.: Effect of the Range of Interactions on the Properties of Polar and Associating Fluids: Phase Equilibria and Structure. 2002 Annual AIChE Meeting, p. 50g, Indianapolis IN, USA, 03-08 November 2002.
44. Chialvo A.A., Předota M., Cummings P.T.: Electric Double Layer in Hydrothermal Systems. Molecular Simulation and Experiment. 2002 Annual AIChE Meeting, p. 50g, Indianapolis IN, USA, 03-08 November 2002.

45. Colina C.M., Olivera-Fuentes C.G., Lísal M., Siperstein F.R., Gubbins K.E.: Thermal Properties of Carbon Dioxide in the Single-Phase Region by Monte Carlo Simulations. 2002 Annual AIChE Meeting, p. 51c, Indianapolis IN, USA, 03-08 November 2002.
46. Cummings P.T., Předota M., Chialvo A.A.: Molecular-Based Study of the Electric Double Layer in Hydrothermal Systems. 12th Annual V.M. Goldsmith Conference, p. A160, Davos, Switzerland, 18-23 August 2002.
47. Kolafa J.: Molecules Dynamics of Potential Models with Polarizability: Comparison of Methods. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
48. Kolafa J.: The Bridge Function of Hard Spheres by Direct Inversion of Computer Simulation Data. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
49. Linek J., Morávková L.: Temperature Dependence of Excess Molar Volumes of the Systems Heptane + 1-Chloroalkane and Octane + 1-Chloroalkane. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 319, Prague, Czech Republic, 25-29 August 2002.
50. Linek J., Morávková L.: P-V-T Behaviour of Liquid Alkane - 1-Chloroalkane Mixtures at Elevated Temperatures and High Pressures. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 109, Prague, Czech Republic, 25-29 August 2002.
51. Lísal M., Smith W.R.: New Direct Monte Carlo Simulation Methods for Non-reacting and Reacting Systems at Fixed Total Internal Energy or Enthalpy. 19th European Seminar on Applied Thermodynamics ESAT 2002, Proceedings, p. 161-162, Santorini, Greece, 06-10 September 2002.
52. Lísal M., Smith W.R.: Direct Monte Carlo Simulation Methods for Nonreacting and Reacting Systems at Fixed Total Internal Energy or Enthalpy. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
53. Morávková L., Linek J.: Excess Molar Volumes of the Octane-1-Chlorobutane System at Elevated Temperatures and High Pressures. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 30, Tatranské Matliare, Slovakia, 27-31 May 2002.
54. Morávková L., Linek J.: Temperature Dependence of the Excess Molar Volume of the Octane-1-Chloroalkane Systems. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 132, Tatranské Matliare, Slovakia, 27-31 May 2002.
55. Nezbeda I.: Modeling of Aqueous Electrolytes at the Molecular Level: On the Origin of the Structure Breaking and Structure Enhancement Phenomena. 17th IUPAC Conference on Chemical Thermodynamics, Rostock, Germany, 28 July - 02 August 2002.
56. Nezbeda I.: Towards a Unified View of Fluids. Liquid Matter Conference, Konstanz, Germany, 14-18 September 2002.
57. Nezbeda I.: Towards a Unified View of Fluids. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
58. Pavlíček J., Aim K.: Perturbation Theory for Fluids of Polar and Polarizable Convex Molecules: Application to Linear Chloroalkanes and Their Mixtures with n-Alkanes. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
59. Předota M., Chialvo A.A., Cummings P.T.: Molecular Dynamics Simulation of Aqueous Systems at TiO₂ Surfaces. American Chemical Society Spring Meeting, Orlando FL, USA, 07-11 April 2002.

60. Předota M., Chialvo A.A., Cummings P.T.: Molecular Simulation Study of the Metal Oxide/Fluid Interface on Hydrothermal Systems Involving Ab Initio Derived Intermolecular Potentials. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
61. Předota M., Chialvo A.A., Cummings P.T.: Nanoscale Phenomena at Metal Oxide Surfaces. 2002 Annual AIChE Meeting, p. 8f, Indianapolis IN, USA, 03-08 November 2002.
62. Slovák J., Nezbeda I.: Adsorption of Fluids of Pseudo-Hard Bodies and EPM 5 Water on Solid Surface: Density Functional Theory. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
63. Smith W.R., Lísal M.: Direct Monte Carlo Simulation Methods for Nonreacting and Reacting Systems at Fixed Enthalpy or Internal Energy. 2002 Annual AIChE Meeting, p. 397c, Indianapolis IN, USA, 03-08 November 2002.
64. Smith W.R., Lísal M.: New Monte Carlo Simulation Methodology for Reacting and Systems at Fixed Internal Energy or Enthalpy. 52nd Canadian Chemical Engineering Conference, Vancouver BC, Canada, 20-23 October 2002.
65. Vlček L., Nezbeda I.: Size and Shape Dependence of Hydrophobic Hydration. 6th Liblice Conference on Statistical Mechanics of Liquids, Špindlerův Mlýn, Czech Republic, 09-14 June 2002.
66. Wagner Z.: Evaluation of High-Pressure Vapour-Liquid Equilibrium Data by Means of Gnostic Theory. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 286, Prague, Czech Republic, 25-29 August 2002.
67. Wagner Z., Ždímal V., Smolík J.: Application of Gnostic Theory to Analysis of Particle Size Distribution. Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56, pp. 164-168, Prague, Czech Republic, 23-26 May 2002.
68. Wichterle I.: Generalization of EOS Parameters in Systems Containing CO₂ at High Pressures. XIV International Conference on Chemical Thermodynamics, Abstracts, p. 313, St. Petersburg, Russia, 01-05 July 2002.
69. Wichterle I.: Interaction Parameters for the R-K-S Equation of State in Some Binary Systems at High Pressures. 3rd International Conference of the Chemical Societies of the South-Eastern European Countries, Book of Abstracts, OP121, p. 150, Bucharest, Romania, 22-25 September 2002.
70. Wichterle I., Aim K.: Phase Equilibria in Three Systems with Esterification Reaction. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 123, Prague, Czech Republic, 25-29 August 2002.
71. Wichterle I., Linek J., Wagner Z., Kehiaian H.: Vapor-Liquid Equilibrium in Mixtures and Solutions Bibliographic Database. XIV International Conference on Chemical Thermodynamics, Abstracts, p. 507, St. Petersburg, Russia, 01-05 July 2002.

Department of Catalysis and Reaction Engineering

Head: M. Zdražil
Deputy: P. Schneider
Research staff: J. Cinibulk, D. Gulková, V. Hejtmánek, K. Jirátová, L. Kaluža, T. Klicpera, J. Kociánová, R. Ponec, H. Šnajdaufová, O. Šolcová, Z. Vít
Technical staff: H. Součková, G. Yuzhakov
PhD students: P. Čuba, J. Rymeš, K. Soukup

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

Applied research

- Catalytic combustion of volatile organic compounds
- Textural characteristics of structural materials

Research projects

Complex textural characterisation of porous solids regarding the mutual relationship of different methods

(O. Šolcová, supported by GA ASCR, grant No. 4072915)

The standard textural analysis methods (the nitrogen physisorption, mercury porosimetry, helium pycnometry, and liquid-expulsion permoporometry) and non-standard transport measurement methods (multicomponent counter-current isobaric diffusion, gas permeation under non-steady state conditions) are applied for complex analysis of pore structure of a broad set of industrial porous solids (monodisperse pore-size distributions, bi- and polydisperse pore-size distributions, with micropores, mesopores and macropores, etc.). The correlation of data obtained from all methods allows a novel approach in determination and prediction of transport parameters characterising processes taking place in porous solids (porous heterogeneous catalysts, membranes, adsorbents, zeolites, etc.). [Refs. 9, 18, 19, 30, 49, 51, 53]

Correct characterisation of porous solids for mass transport in pores

(O. Šolcová, supported by GA CR, grant No. 104/01/0546)

The project develops and proves the methods for obtaining material constants of porous solids for the description of mass transport in pores (transport parameters) from standard textural analyses (physical adsorption, mercury porosimetry, permeometry). The new counter-current diffusion set-up is designed and constructed. The Graham law is used for description and data evaluation from multicomponent counter-current isobaric diffusion. Verification of the validity of Graham law in porous solids with wide range of pore sizes (from nanometers to tenth and hundredth of micrometers) forms a significant part of the project. [Refs. 3, 15, 22, 23, 25, 31, 50, 52]

Molybdenum sulfide catalysts promoted by platinum metals

(Z. Vít, supported by GA ASCR, grant No. A4072103)

An Mo/alumina catalyst was modified by small amounts (<0.8 mass %) of well-dispersed platinum metals of the 2nd and 3rd row (Pd, Pt, Ru, Rh, Ir). Variables such as the way of catalyst preparation, type of platinum metal or effect of H₂S addition to the feed were studied in attempts to improve activity of the Mo phase or to achieve promotional behavior. Catalytic properties were evaluated in hydrodesulfurization (HDS) and hydrodenitrogenation (HDN) of model compounds (thiophene and pyridine). Addition of all platinum metals had positive effect on activity of Mo catalyst. Synergetic effects of about 3-7 were observed either in HDS or in HDN. The effect of platinum metal was influenced by preparation procedure and by position of the metal in periodic system. The addition of Rh, Ru and Pd improved mainly HDS, while addition of Ir or Pt was more selective to HDN. [Refs. 2, 16, 18, 32, 33, 34]

Catalytic combustion of volatile organic compounds

(K. Jiráťová, supported by GA ASCR, grant No. A4072904)

Activity and selectivity of supported Pt catalysts prepared from reverse microemulsions were examined in catalytic combustion of model organic compounds (toluene, ethanol). It was confirmed that the size of Pt, distribution of Pt throughout the catalyst pellets and catalytic activity are affected by the conditions of microemulsion preparation. With higher viscous microemulsions used during preparation, more active catalysts are prepared. [Refs. 13, 14, 40, 47, 48]

Physico-chemical properties and catalytic activities of supported catalysts based on phosphomolybdic acids

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

Alumina supported hydrotreating catalysts prepared from phosphotungstic acid and Fe salts of phosphomolybdic acids were examined in hydrodesulfurization of thiophene and the activities were correlated with reducibility and acid-base properties of the catalysts. [Refs. 25, 27]

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

(K. Jiráťová, supported by GA CR, grant No. 106/02/0523)

Reducibility and acid-base properties of various calcined hydrotalcite-like compounds (Ni/Mn/Mg/Al, Ni/Al, Co/Al, Cu/Al, Mg/Al) were examined by TPR and TPD of CO₂ and NH₃. The systems containing two or more transition metals are reduced in two waves, the lower having direct connection with catalytic activity. Basicity increased, and acidity decreased, with increasing amount of magnesium in the catalysts. [Refs. 4, 36, 37, 45]

Sulfide hydrotreating catalysts with unconventional supports

(M. Zdražil, supported by GA CR, grant No. 104/01/0544)

Highly active CoMo and NiMo sulfide hydrodesulfurization catalysts supported over MgO were prepared by new method of non-aqueous impregnation [Refs. 8, 35]. Organized mesoporous alumina was used as a new support of Mo sulfide catalyst. Very high loading of 30 mass% of MoO₃ was effectively dispersed using this support. The catalysts exhibited high activity in hydrodesulfurization of thiophene [Refs. 1, 7]. The Mo/Al₂O₃ catalysts with sharp eggshell Mo distribution were prepared by the reaction of Al₂O₃ extrudates with slurry of MoO₃ in water. The radial profiles of Mo concentration were almost rectangular and the Mo concentration in the shell corresponded to saturated monolayer. The thickness of the shell was easily regulated by the amount of MoO₃ used [Refs. 6, 41, 42, 43]. CoMo/C hydrodesulfurization catalysts were prepared by the reaction of Mo/C catalyst with the slurry of cobalt hydroxycarbonate in water. The Co species deposited in that way exhibited higher promotion effect in activity as compared with Co species deposited by conventional impregnation [Ref. 5].

Role of electron pairing in chemical bonds

(R. Ponec, supported by GA ASCR, grant No. A4072006)

The project deals with the theory of chemical bond, especially in the evaluation of the role of electron pairing in chemical bonding. For this purpose, a new procedure, based on the analysis of the so-called domain averaged Fermi hole, was recently proposed. The approach was applied to the elucidation of bonding in several molecules containing complex bonding patterns like the multicenter bonds, hypervalence, etc. [Refs. 11, 12, 20, 21, 28]

Design of theoretical QSAR models based on quantum similarity data

(R. Ponec, supported by Ministry of Education, grant No. D09.20)

The project deals with the theoretical approach to the design of new structure-activity relationships based on the systematic use of similarity measures and indices as new theoretical descriptors. The project is solved in the collaboration with the Institute of Computation Chemistry of the University of Girona. [Refs. 10, 17, 29]

International co-operations

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

University of Hannover, Hannover, Germany: Analysis of the pair density matrix

University of Buenos Aires, Buenos Aires, Argentina: Analysis of the pair density matrix

Institute of Computation Chemistry, University of Girona, Spain: Analysis of the pair density matrix

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

University of Strasbourg, France: Characterisation and catalytic behaviour of supported catalysts containing precious metals and/or transition metal oxides used in combustion of VOC

Institute of Catalysis, Sofia, Bulgaria: Active phase-support interactions in the catalysis of the hydrotreating and oxidation reactions

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

Visits abroad

T. Klicpera: University of Tokyo, Tokyo, Japan (12 months)

Visitors

D.L. Cooper, University of Liverpool, Liverpool, Great Britain

L. Lain, University of Pais Vasco, Bilbao, Spain

N. Allan, University of Bristol, Bristol, Great Britain

Teaching

K. Jiráťová: ICT, postgraduate course "Preparation of heterogeneous catalysts"

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

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

M. Zdražil: ICT, postgraduate course "Preparation of heterogeneous catalysts"

Publications

Original papers

1. Čejka J., Žilková N., Kaluža L., Zdražil M.: Mesoporous Alumina as a Support for Hydrodesulfurization Catalysts. *Stud. Surf. Sci. Catal.* 141, 243-250 (2002).
2. Cinibulk J., Vít Z.: Preparation of Mo/Al₂O₃ Sulfide Catalysts Modified by Ir Nanoparticles. *Stud. Surf. Sci. Catal.* 143, 443-451 (2002).
3. Hudec P., Smieskova A., Zídek Z., Schneider P., Šolcová O.: Determination of Microporous Structure of Zeolites by t-plot Method – State-of-the-Art. *Stud. Surf. Sci. Catal.* 142, 1587-1594 (2002).
4. Jiráťová K., Čuba P., Kovanda F., Hilaire L., Pitchon V.: Preparation and Characterisation of Ni(Mn)/Mg/Al Hydrotalcites for Combustion Catalysis. *Catal. Today* 76(1), 43-53 (2002).
5. Kaluža L., Zdražil M.: Preparation of Mo-S/C and Co-Mo-S/C Catalysts by Slurry Impregnation. *Petroleum and Coal* 43(3-4), 198-207 (2002).
6. Kaluža L., Zdražil M.: Preparation of MoO₃/Al₂O₃ Catalysts with Sharp Eggshell Mo Distribution by Slurry Impregnation. *Catal. Lett.* 78(1-4), 313-318 (2002).
7. Kaluža L., Zdražil M., Žilková N., Čejka J.: High Activity of Highly Loaded MoS₂ Hydrodesulfurization Catalysts Supported on Organised Mesoporous Alumina. *Catal. Commun.* 3, 151-157 (2002).
8. Klicpera T., Zdražil M.: Preparation of High-Activity MgO-Supported Co-Mo and Ni-Mo Sulfide Hydrodesulfurization Catalysts. *J. Catal.* 206(2), 314-320 (2002).
9. Novák P., Brabec L., Šolcová O., Bortnovsky O., Zikánová A., Kočířik M: Square Root Relationship in Growth Kinetics of Silicalite-1 Membranes. *Stud. Surf. Sci. Catal.* 142, 1505-1511 (2002).

10. Ponec R., Gironés X., Carbó-Dorca R.: Molecular Basis of Linear Free Energy Relationships. The Nature of Inductive Effect in Aliphatic Series. *J. Chem. Inf. Comput. Sci.* 42(3), 564-570 (2002).
11. Ponec R., Gironés X.: Chemical Structures from the Analysis of Domain-Averaged Fermi Holes. Hypervalence and the Nature of Bonding in Isoordinated Molecules SF₆ and CLi₆. *J. Phys. Chem.* 106, 9506-9511 (2002).
12. Ponec R., Roithová J., Gironés X., Lain L., Torre A., Bochicchio R.: On the Nature of C-Li Bonding in Lithiated Hydrocarbons and Lithiocarbons. *J. Phys. Chem. A* 106(6), 1019-1025 (2002).
13. Rymeš J., Ehret G., Hilaire L., Boutonnet M., Jirátová K.: Microemulsions in the Preparation of Highly Active Combustion Catalysts. *Catal. Today* 75(1-4), 297-303 (2002).
14. Rymeš J., Ehret G., Hilaire L., Jirátová K.: Pt Combustion Catalysts Prepared from W/O Microemulsions. *Stud. Surf. Sci. Catal.* 143, 121-129 (2002).
15. Šolcová O., Schneider P.: Transport Characteristics of Porous Solids Derived from Chromatographic Measurements. *Stud. Surf. Sci. Catal.* 144, 475-482 (2002).
16. Vít Z., Cinibulk J.: Effect of H₂S on Pyridine HDN over Ir, Mo and Ir-Mo/Al₂O₃ Sulfide Catalysts. *React. Kinet. Catal. Lett.* 77(1), 43-49 (2002).
17. Amat L., Carbó-Dorca R., Cooper D.L., Allan N.L., Ponec R.: Structure-Property Relationships and Momentum Space Quantities: Hammett Sigma Constants. *Mol. Phys.*, in press.
18. Cinibulk J., Gulková D., Yoshimura Y., Vít Z.: Effect of Preparation of the Ir-Mo/Al₂O₃ Sulfide Catalyst on HDS and HDN Activity. *Appl. Catal., A*, submitted.
19. Pavlů J., Kudová J., Zikánová A., Kočířik M., Uchtyl P., Šolcová O., Roček J., Fíla V., Bernauer B., Krystl V., Hrabánek P.: Keramické porézní elementy pro filtraci plynů a příbuzné aplikace. (Czech) Ceramic Porous Elements for Gas Separation and Related Applications. *Chem. Listy*, in press.
20. Ponec R., Cooper D.: Generalized Population Analysis of Three-Center Two-Electron Bonding. *Phys. Chem. Chem. Phys.*, submitted.
21. Ponec R., Juzakov G., Cooper D.: Electron Reorganization in Chemical Reactions. Structural Changes from the Analysis of Bond Order Profiles. *J. Phys. Chem.*, submitted.
22. Šolcová O., Schneider P.: Multicomponent Counter-Current Gas Diffusion: Determination of Transport Parameters. *Appl. Catal., A*, in press.
23. Šolcová O., Schneider P.: Axial Dispersion in Single Pellet-String Columns with Non-Porous Packing. *Chem. Eng. Sci.*, submitted.
24. Šolcová O., Schneider P.: Application of Liquid-Expulsion Perm-Porometry (LEPP) to Commercial and Model Porous Solids. *Appl. Catal., A*, submitted.
25. Spojakina A.A., Jirátová K., Kostova N.G., Kociánová J., Stamenova M.: Tungsten Hydrotreating Catalysts I. Countercation Effect on the Properties of Alumina Supported 12-PW₁₂O₄₀. *J. Mater. Sci.*, in press.
26. Spojakina A.A., Kostova N.G., Vít Z., Zdražil M.: MoO₃/Al₂O₃ Catalyst: Comparison of Catalysts Prepared by New Slurry Impregnation with Molybdic Acid with Conventional Samples. *Pol. J. Chem.*, in press.
27. Spojakina A.A., Králeva E.U., Jirátová K., Kociánová J., Petrov L.A.: FePMo₁₂O₄₀ Heteropolycompounds in Preparation of Hydrodesulfurization Catalysts. *Bulgar. Chem. Commun.*, submitted.
28. Torre A., Lain L., Bochicchio R., Ponec R.: Topological Population Analysis from Higher Order Densities II. The Correlated Case. *J. Math. Chem.*, in press.

Chapters in books

29. Girones 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.
30. 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

31. Čapek P., Hejtmánek V.: A Limited Benefit of the Wicke-Kallenbach Cell for the Study of the Mass Transport Dynamics. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 144, Tatranské Matliare, Slovakia, 27-31 May 2002.
32. Cinibulk J., Vít Z.: Effect of Ir Loading and Sulfur Compounds on Hydrodenitrogenation Activity of the Ir-Mo/Alumina Sulfide Catalyst. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 291, Praha, Czech Republic, 25-29 August 2002.
33. Cinibulk J., Vít Z., Gulková D.: MoS₂/Al₂O₃ Catalyst Promoted by Noble Metals: Effect of Kind of Noble Metal. XXXIV Symposium on Catalysis, Book of Abstracts, p. 43, Praha, Czech Republic, 04-05 November 2002.
34. Cinibulk J., Vít Z., Gulková D., Yoshimura Y.: Mo/Al₂O₃ Catalyst Promoted by Ir Nanoparticles. Effect of Sulfidation on the Mo Matrix. XXXIV Symposium on Catalysis, Book of Abstracts, p. 72, Praha, Czech Republic, 04-05 November 2002.
35. Cinibulk J., Vít Z., Klicpera T., Zdražil M.: Magnesia Supported-Mo, NiMo and CoMo Sulfide Hydrodesulfurization and Hydrodenitrogenation Catalysts. 6th Pannonian International Symposium on Catalysis, Book of Abstracts, p. 152, Obergurgl, Ötztal, Austria, 11-14 September 2002.
36. Čuba P., Kovanda F., JirátoVá K.: Properties and Catalytic Activity of Calcined Hydrotalcite like Compounds. 6th Pannonian International Symposium on Catalysis, Book of Abstracts, p. 162-163, Obergurgl, Ötztal, Austria, 11-14 September 2002.
37. Čuba P., Kovanda F., JirátoVá K.: Activity of Calcined Hydrotalcite-like Compounds in Catalytic Combustion of Volatile Organic Compounds (VOC). 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 5, p. 312, Prague, Czech Republic, 25-29 August 2002.
38. Gulková D., Šolcová O., Klicpera T., Zdražil M.: Preparation, Texture and Stability of High Surface Area MgO Support and MoO₃/MgO Catalyst. 6th Pannonian International Symposium on Catalysis, Book of Abstracts, p. 158-159, Obergurgl, Ötztal, Austria, 11-14 September 2002.
39. Gulková D., Šolcová O., Klicpera T., Zdražil M.: Comparison of High Surface Area MgO with Al₂O₃ Support. XXXIV Symposium on Catalysis, Book of Abstracts, 11, p. 46, Prague, Czech Republic, 04-05 November 2002.
40. JirátoVá K., Ioannides T., Čuba P., Avgouropoulos G., Kociánová J.: Influence of Acid-Base Properties of Modified Alumina on VOC Combustion Activity of Pt/Al₂O₃ Catalyst. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 341, Prague, Czech Republic, 25-29 August 2002.
41. Kaluža L., Zdražil M.: Preparations of Hydrotreating Catalysts with Eggshell and Uniform Mo Distribution by a New Slurry Impregnation Method. 2002 Younger

- European Chemists' Conference, Posters, 49, Heidelberg, Germany, 30 September - 02 October 2002.
42. Kaluža L., Zdražil M.: Application of Slurry Impregnation for Preparation of $\text{MoO}_3/\text{Al}_2\text{O}_3$ Catalysts with Sharp Eggshell Mo Distribution. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 278, Prague, Czech Republic, 25-29 August 2002.
 43. Kaluža L., Zdražil M.: Preparation of Hydrotreating Catalysts with Eggshell and Uniform Mo Distribution by a New Slurry Impregnation Method. XXXIV Symposium on Catalysis, Book of Abstracts, p. 49, Praha, Czech Republic, 04-05 November 2002.
 44. Lain L., Torre A., Bochichio R., Ponec R.: Analisis de poblacion de la matriz densidad de electrones efectivamente desapareados. (Span) Population Analysis of the Matrix of Effectively Unpaired Electrons. QXXVIII Congreso de Quimicos Teoricos de Expresion Latina, Book of Abstracts, p. 1, Montevideo, Uruguay, Uruguay, 01-08 September 2002.
 45. Obalová L., Kovanda F., JirátoVá K., Chmielová M., Wichterle K., Dorničák V.: Catalytic Decomposition of Nitrous Oxide over Calcined Hydrotalcite-like Compounds. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 356, Prague, Czech Republic, 25-29 August 2002.
 46. Ponec R., Gironés X.: Nature of Bonding in SF_6 and CLi_6 from the Analysis of Domain Averaged Fermi Holes. The 17th Dubrovnik International Course and Conference on the Interface between Mathematics, Chemistry and Computer Sciences, Book of Abstracts, p. 60, Dubrovnik, Croatia, 24-29 June 2002.
 47. Rymeš J., Ehret G., Hilaire L., JirátoVá K.: Effect of W/O Microemulsion Properties on Activity of Pt Combustion Catalysts. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 5, p. 311, Prague, Czech Republic, 25-29 August 2002.
 48. Rymeš J., JirátoVá K., Ehret G., Hilaire L.: Activity and Selectivity of Pt Combustion Catalysts Prepared from w/o Microemulsions. XXXIV Symposium on Catalysis, p. 61-62, Prague, Czech Republic, 04-05 November 2002.
 49. Šolcová O., Schneider P.: Transport Characteristics of Porous Solids from Chromatographic Peaks. 6th International Symposium on the Characterization of Porous Solids, Abstracts, p. P66, Alicante, Spain, 08-11 May 2002.
 50. Šolcová O., Schneider P.: Chromatographic Determination of Transport Characteristics of Porous Solids. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 17, Prague, Czech Republic, 25-29 August 2002.
 51. Šolcová O., Šnajdaufová H., Schneider P.: Multicomponent Counter-Current Gas Diffusion; Transport Parameter Determination. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 146, Tatranské Matliare, Slovakia, 27-31 May 2002.
 52. Šolcová O., Součková H., Schneider P.: Transport Characteristics of Porous Solids from Chromatographic Methods. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 145, Tatranské Matliare, Slovakia, 27-31 May 2002.
 53. Šolcová O., Uchytíl P., Schneider P.: Textural Properties of Porous Solids from Liquid Expulsion Permporometry. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 343, Prague, Czech Republic, 25-29 August 2002.
 54. Torre A., Lain L., Bochicchio R., Ponec R.: Estudios de análisis de población topológico de densidades de alto orden, a nivel de correlación. (Span) Study of the Topological Population Analysis of Higher Order Densities at Correlated Level. QXXVIII Congreso de Quimicos Teoricos de Expresion Latina, Book of Abstracts, p. 1, Montevideo, Uruguay, 01-08 September 2002.

Department of Multiphase Reactors

Head: J. Drahoš
Deputy: J. Tihon
Research staff: M. Fialová, M. Růžička, J. Slezák, V. Sobolík, O. Wein
Part time: V. Pěnkavová, M. Plzánková
Technical staff: S. Nováková, V. Tovchigrechko
PhD students: M. Večeř, J. Vejražka

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 flow

Research projects

Instability of homogeneous flow regime in bubble columns

(M. Růžička, supported by GA CR, grant No. 104/01/0547)

Studies on homogeneous-heterogeneous flow regime transition in gas-liquid bubble columns. Identification of the hydrodynamic mechanism responsible for the instability of the homogeneous flow regime. Investigation of the instability character. [Refs. 10, 11, 13, 22-35]

Rheometric and electrodiffusion study of the apparent wall slip in lyophobic dispersions

(O. Wein, supported by GA CR, grant No.104/01/0545)

Apparent wall slip in several water-soluble polysaccharides was studied experimentally, using rotational viscometry. An extensive collection of the related material functions has been obtained. Viscometric theory was developed for a novel rotational viscometer with coaxial Morse cones. [Ref. 4, 40, 46, 48]

Mixing of concentrated suspensions

(V. Sobolík, joint project with CTU, Faculty of Mechanical Engineering, Prague, supported by GA CR, grant No. 101/02/0615)

The goal of the project focused on mixing of concentrated suspensions is: - To work out an objective methodology based on electrochemical method that will enable to investigate the course of particle suspension and to determine the critical impeller speed required to achieve off-bottom suspension for particles of various densities. - To propose dimensionless relations describing the course of particle suspension in the mixing equipments with different geometries. [Refs. 1, 3, 6]

Electrochemical sensors for flow measurements

(J.Tihon, COST project supported by the Ministry of Education, OC F2.10/1996)

Electrochemical technique for the near-wall flow diagnostics has been improved (sensors manufacturing, development of the control electronics, dynamic response of the sensors). The directionally sensitive segment probes have been applied to study different flow situations (near-wall turbulence, backward-facing step flow, Taylor-Couette flow, impinging fluid jet, wavy film flow). [Refs. 1, 3, 6, 7, 14, 36, 38, 39, 41-45]

Flow regimes and mass-transfer in two-phase chemical reactors

(O.Wein, grant for the Marie Curie Training Sites, supported by the Commission of the European Communities under contract HPMT-CT-2000-00074 within the program "Improving Human Potential and the Socio-Economic Knowledge Bases")

The project gives young researchers pursuing doctoral studies the opportunity to receive training within diagnostics of multiphase flows. One PhD student stayed in our laboratory during last year.

Research Centre: Behaviour of multiphase systems under superambient conditions

(J. Drahoš, I. Wichterle, supported by EU 5th RTD NAS2 72074)

This interdisciplinary Research Centre (BEMUSAC) integrates physical chemists and chemical engineers to study and develop new processes based on gas-liquid-solid contacting. It has been established in view of significant reorientation and transformation of the R&D potential towards the advanced fields of multiphase systems under extreme conditions, namely to thermodynamic systems at high pressures and temperatures, to bubble processes in metallurgy and to hydrodynamics of rheologically complex systems.

International co-operations

UMIST, Manchester, Great Britain: Gas-liquid reactors for complex rheology fluids

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

CNRS UPR 15, Paris, France: Electrodiffusion diagnostics of flow

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

LEGI / IMG, Grenoble, France: Impinging jets

University of Poitiers, France: Electrochemical sensors for flow measurements

Institute of Chemical Engineering of BAS, Sofia, Bulgaria: Gas-liquid reactors for complex rheology fluids

Swiss Federal Institute of Technology, Lausanne, Switzerland: Hydrodynamics of bubbly flow

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

University of Thessaly, Volos, Greece: Liquid film flows

Visits abroad

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

J. Vejražka: LEGI / IMG, Grenoble, France (7 months)

Visitors

D. Bröder, Martin Luther Universität, Halle, Germany (3 months)

P. Crausse, Institute of Fluid mechanics, Toulouse, France

N.D. Kovalevskaya, ITMO Minsk, Belorussia

Teaching

J. Drahoš: ICT, course "Fluid Mechanics" and postgraduate courses "Multiphase reactors", "Time series analysis in chemical engineering" and "Applied statistical analysis and data processing"

M. Fialová: ICT, 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. Barbeau F., Sobolík V., Martemianov S., Gbahoue L.: Caractéristique directionnelle calculée et mesurée d'une sonde électrochimique. (Fr) Calculated and Measured Directional Characteristic of an Electrochemical Probe. *C. R. Mecanique* 330(6), 433-436 (2002).
2. Drahoš J., Punčochář M.: Comments on Application of the Fractional Brownian Motion in an Airlift Reactor. *Chem. Eng. Sci.* 57(10), 1831-1832 (2002).
3. Dumont E., Fayolle F., Sobolík V., Legrand J.: Wall Shear Rate in the Taylor-Couette-Poiseuille Flow at Low Axial Reynolds Number. *Int. J. Heat Mass Transfer* 45(3), 679-689 (2002).
4. Elgozali A., Linek V., Fialová M., Wein O., Zahradník J.: Influence of Viscosity and Surface Tension on Performance of Gas-Liquid Contactors with Ejector Type Gas Distributor. *Chem. Eng. Sci.* 57(15), 2987-2994 (2002).
5. Sobolík V., Žitný R., Tovčigrečko V., Delgado M., Allaf K.: Viscosity and Electrical Conductivity of Concentrated Solutions of Soluble Coffee. *J. Food Eng.* 51(2), 93-98 (2002).
6. Tihon J.: Electrodiffusion Diagnostics of the Near-Wall Flows. *Chem. Pap.* 56(1), 45-51 (2002).
7. Vejražka J., Marty P., Sobolík V.: Heat Transfer Experiments in a Submerged Impinging Round Jet Using Liquid Crystal Thermometry. *Int. J. Heat Technol.* 20(1), 45-50 (2002).
8. Vrba J.: Basic Aspects of Uncertainty I. The Membership Characteristics Transfer. *SAMS* 42, 1219-1252 (2002).
9. Vrba J.: Basic Aspects of Uncertainty II. The Inverse Estimations. *SAMS* 42, 1253-1269 (2002).
10. Fialová M., Růžička M., Drahoš J.: Factors Influencing Character of Bubble Bed in Bubble Column Reactors. *Can. J. Chem. Eng.*, submitted.

11. Höller V., Růžička M., Renken A., Drahoš J.: Acoustic and Visual Study of Bubble Formation Processes in Bubble Columns Staged with Fibrous Catalytic Layers. *Catal. Today*, submitted.
12. Punčochář M., Drahoš J.: Entropy of Fluidized Bed - a Measure of Particle Mixing. *Chem. Eng. Sci.*, submitted.
13. Růžička M., Thomas N.H.: Buoyancy-Driven Instability of Bubbly Layers: Analogy with Thermal Convection. *Int. J. Multiphase Flow*, in press.
14. Tihon J., Tovčigřečko V., Sobolík V., Wein O.: Electrodiffusion Detection of the Near-wall Flow Reversal in Liquid Films at the Regime of Solitary Waves. *J. Appl. Electrochem.*, submitted.
15. Vejražka J., Marty P.: Measurement of Temperature Field Using Thermochromic Liquid Crystals. *Int. J. Thermal Sci.*, submitted.
16. Vlaev S.D., Fialová M.: Bubble Column Bioreactors: Comparison with Stirred Fermenters Based on Local Gas Hold-up Distribution. *Can. J. Chem. Eng.*, submitted.
17. Wein O., Tihon J.: Linear Stability of Inclined Film Flows. *Fluid Dyn. Res.*, submitted.

Chapters in books

18. Drahoš J., Punčochář M.: Fraktály a chaos: další z vědeckých revolucí 20. století? (Czech) Fractals and Chaos: Another 20th Century Scientific Revolution? In: *Myšlenky na zlomu tisíciletí. (Czech) Thoughts for the New Millennium* (Mizerová, A. - Sedlák, J. - Dub, P., Eds.), pp. 255-277, VUTIUM, Brno 2002.

Patents

19. Hájek M., Drahoš J.: Způsob vysoušení a desinfekce knih a papírových materiálů. (Czech) Method of Drying and Desinfection of Books and Paper Materials. Pat. No. PV2002-4272. Applied: 02.12.30.
20. Hájek M., Drahoš J.: Způsob a zařízení pro kontinuální výrobu vláken z přírodních surovin zvláště vulkanického původu. (Czech) Method and Equipment for Continuous Production of Fibers of Volcanic Origin. Pat. No. PV2002-33428. Applied: 02.10.16.
21. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Volcanic Origin. PCTI/CZ00/00042/ (in press).

Conferences

22. Bröder D., Růžička M., Drahoš J., Sommerfeld M.: High-Speed Video Images of Hydrodynamic Interactions in Bubbly Flow. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 221, Prague, Czech Republic, 25-29 August 2002.
23. Dostál P., Růžička M., Drahoš J., Wichterle K.: Acoustic Emissions from Bubble Columns. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 180, Tatranské Matliare, Slovakia, 27-31 May 2002.
24. Dostál P., Růžička M., Drahoš J., Wichterle K.: Acoustics of Bubble Formation: a Preliminary Study. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 217, Prague, Czech Republic, 25-29 August 2002.
25. Fialová M.: Effect of Liquid Phase Viscosity and Type of Gas Distributor on Gas Phase Mixing in Bubble Column Reactor. 15th International Congress of Chemical and Process

- Engineering CHISA 2002, Summaries 1, p. 308-309, Prague, Czech Republic, 25-29 August 2002.
26. Fialová M., Zahradník J., Růžička M., Drahoš J., Řezníčková J.: Effect of Gas Distributor and Column Geometry on Bubbling Regimes and Gas Holdup in Bubble Column Reactors. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 337-338, Prague, Czech Republic, 25-29 August 2002.
 27. Hoeller V., Růžička M., Renken A., Drahoš J.: Staged Bubble Columns with Hydrophones and High-Speed Video. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 220, Prague, Czech Republic, 25-29 August 2002.
 28. Hoeller V., Růžička M., Renken A., Drahoš J.: Staged Bubble Columns: A Preliminary Visual and Acoustic Study. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 181, Tatranské Matliare, Slovakia, 27-31 May 2002.
 29. Höller V., Růžička M., Drahoš J., Kivi-Minsker L., Renken A.: Acoustic and Visual Study of Bubble Formation Processes in Bubble Columns Staged with Fibrous Catalytic Layers. 4th International Symposium Catalysis in Multiphase Reactors, Call for Papers, Lausanne, Switzerland, 22-25 September 2002.
 30. Mena P., Růžička M., Drahoš J., Teixeira J., Rocha F.: Effect of Viscosity on Flow Regime Transition in Bubble Columns. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 219, Prague, Czech Republic, 25-29 August 2002.
 31. Mena P., Růžička M., Drahoš J., Teixeira J., Rocha F.: Effect of Viscosity on Homogeneous Regime Stability in Bubble Columns. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 183, Tatranské Matliare, Slovakia, 27-31 May 2002.
 32. Mena P., Růžička M., Drahoš J., Teixeira J., Rocha F.: Effect of Surfactants on Homogeneous Regime Stability in Bubble Column. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 182, Tatranské Matliare, Slovakia, 27-31 May 2002.
 33. Mena P., Růžička M., Drahoš J., Teixeira J., Rocha F.: Effect of Surface Active Agents on Flow Regime Transition in Bubble Columns. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 218, Prague, Czech Republic, 25-29 August 2002.
 34. Růžička M., Bröder D., Drahoš J., Sommerfeld M.: Visual Study of Bubble-Bubble Interactions with High-Speed Camera. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 179, Tatranské Matliare, Slovakia, 27-31 May 2002.
 35. Sommerfeld M., Bröder D., Růžička M., Drahoš J.: Modelling Bubble Collisions, Coalescence and Break-Up Using the Lagrangian Approach. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 69, Prague, Czech Republic, 25-29 August 2002.
 36. Tihon J., Deslouis C., Tribollet B.: Structure of the Near-Wall Turbulence in Drag-Reducing Channel Flows Studied by the Electrochemical Technique. 2nd Workshop Local Flow Effects in Hydrodynamic Systems, Book of Abstracts, p. 37, Aachen, Germany, 07-09 November 2002.
 37. Tihon J., Tovčigrečko V.: A New Model Viscoelastic Liquid Based on Water-Slurry Polymers. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 222, Prague, Czech Republic, 25-29 August 2002.

38. Tihon J., Tovčigrečko V., Sobolík V., Wein O.: Electrodifusion Diagnostics of Wavy Films Flow. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 187, Tatranské Matliare, Slovakia, 27-31 May 2002.
39. Tihon J., Tovčigrečko V., Sobolík V., Wein O.: Hydrodynamics of the Solitary Waves Travelling Down a Liquid Film. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 88, Prague, Czech Republic, 25-29 August 2002.
40. Večeř M., Wein O.: Novel Viscometric Configuration for Measuring Apparent Wall-Slip Effect. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 184, Tatranské Matliare, Slovakia, 27-31 May 2002.
41. Vejražka J., Marty P., Tihon J.: Response d'un jet turbulent impactant excite periodiquement. (Fr) Response of a Turbulent Impinging Jet to Periodic Excitation. Congres francais de thermique, SFT 2002, Book of Abstracts, Vittel, France, 03-06 June 2002.
42. Vejražka J., Marty P., Tihon J.: Flow Field of an Exited Impinging Jet. 2nd Workshop Local Flow Effects in Hydrodynamic Systems, Book of Abstracts, p. 29-31, Aachen, Germany, 29-31 November 2002.
43. Vejražka J., Marty Ph.: Measurement of Heat Transfer Coefficient by Thermochromic Liquid Crystals. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 17, Tatranské Matliare, Slovakia, 27-31 May 2002.
44. Vejražka J., Marty Ph., Sobolík V.: Measurement of Temperature Fields Using Thermochromic Liquid Crystals. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 4, pp. 292-293, Prague, Czech Republic, 25-29 August 2002.
45. Vejražka J., Marty Ph., Tihon J.: Experimental Study of Vortex Structures in a Pulsating Impinging Jet. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 47, Prague, Czech Republic, 25-29 August 2002.
46. Wein O., Slezák J., Tovčigrečko V., Večeř V.: A Novel Sensor for Rotational Viscometry under Apparent Wall Slip Effect. 6th European Conference on Rheology EURHEO 2002, Proceedings, 633-634, Erlangen, Germany, 01-06 September 2002.
47. Wein O., Tihon J.: Wavy Films Flow: Linear Stability and Evolution. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 87, Prague, Czech Republic, 25-30 August 2002.
48. Wein O., Večeř M.: A Novel Viscometric Sensor for Measuring the Apparent Wall Slip Effect. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 3, p. 216, Prague, Czech Republic, 25-29 August 2002.

Department of Biotechnology and Environmental Processes

Head: J. Čermák
Deputy: M. Hájek
Research staff: V. Církva, M. Czakóová, J. Hájek, J. Hetflejš, F. Kaštánek, G. Kuncová,
Y. Maléterová, S. Šabata, J. Včelák
Part time: O. Podrazký
Technical staff: J. Brustman, J. Kubešová, Z. Soukup, J. Storch
PhD students: K. Auerová, P. Gavlasová, I. Jurčová, A. Krupková, J. Kurfürstová,
M. Pošta, J. Steinfeld, L. Šťastná, 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
- Detoxification of noxious halogen-containing substances by biochemical dehalogenation
- Microwave-induced catalytic reactions
- Effect of microwave radiation on photochemical reactions
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluoruous biphasic media

Applied research

- Microwave drying of flooded books
- Microwave technology of glass melting
- Complex dehalogenation of PCB contaminated soils, waste water and oils

Research projects

Biodegradation of phenols in water and water sediments

(F. Kaštánek, supported by GA CR, grant No.104/00/0575)

Biodegradation of phenol adsorbed on real (or artificially contaminated) sediments was studied. The efficiency of biodegradation by aerobic oxidation using bacteria strains depends on the size and type of sediment particles and the type of contamination (phenol or mixture of phenol, BTX and PAU). The biodegradation activity was tested using bacteria strains (*Acinetobacter sp.*, *Pseudomonas putida*, *Micrococcus sp.*) and yeast strain *Candida Tropicalis*. Evaluation of laboratory results led to the proposal of bioreactor configuration in a

semi-pilot scale and to the study of the influence of external conditions on the rate of biodegradation. [Ref. 20]

Bioencapsulation innovation and technologies

(G. Kuncová, project supported by COST Action 840 and Ministry of Education)

Research on immobilization of lipase into organic-inorganic matrices has been focused on reduction of the biocatalyst price by partial replacing of poly(methylhydrosiloxane) by the less expensive silicate carrier. A comparative study of lipase activity immobilized by sol-gel process into different organic-inorganic matrices showed that positive effect of hydrophobic-hydrophilic interface, created by the addition of organosilanes, on the activity of biocatalysts was partially reduced by decreasing specific surface of mesopores. [Refs. 6, 13, 36, 37]

Microwave activation of heterogeneous catalytic reactions

(M. Hájek, supported by ICPF)

Research has been focused on microwave activation of heterogeneous catalytic reactions in liquid phase at low temperature (0 to -176 °C). It was found on model reaction of transformation of *tert*-butylphenols that microwaves have a strong effect on reaction rate. The results were explained on the basis of superheating. [Refs. 10, 11, 16, 31]

Microwave technology of glass melting

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

In applied research, a new technology for melting and manufacture of glass by microwave energy has been extended. [Refs. 25, 26]

Effect of microwave radiation on photochemical reactions

(M. Hájek, supported by GA CR, grant No.203/02/0879)

Reactions under simultaneous MW-UV irradiations have been studied using electrodeless UV lamps. [Refs. 23, 35]

Microwave drying of flooded books

(M.Hájek, supported by ICPF)

New technology of microwave drying of flooded books and paper materials have been developed and applied for patent protection. [Ref. 24]

Novel fluorophilic ligands for transition metal complexes based on polyfluorinated alkynes

(J. Čermák, joint project with ICT and CU, supported by GA ASCR, grant No. A4072203)

New silylcyclopentadienyl ligands substituted by polyfluorinated chains were synthesized, together with their mono- and bis(cyclopentadienyl) titanium(IV) complexes. Crystal structure of the unusual titanocene dichloride analogue with fluoros ponytails was determined by X-ray diffraction. New alkene rhodium(I) complexes with previously synthesized (perfluoroalkyl)tetramethylcyclopentadienyl ligands were prepared and studied as homogeneous catalysts for 1-hexyne cyclotrimerization. [Refs. 2, 8, 9, 27]

New highly active catalysts for the Heck reaction

(J. Čermák, joint project with CU, supported by GA CR, grant No. 203/01/0554)

The reaction rate of the Heck reaction catalyzed by various palladium complexes was studied under conditions of standard catalyst loading (0.5 – 1 mol %). Suitable synthetic way of deprotonation of cationic nickel complexes prepared last year was found and crystal structure of the ene-hydrazone complex with bis(dicyclohexylphosphino)-pinacolone azine

was determined by X-ray diffraction. The alternative route to nickel and palladium vinyl complexes starting from alkynes, ligands, and zerovalent metal precursors was studied. [Refs. 1, 41]

Permeable barriers with immobilized bacteria treating mixed pollutants in the environment

(G. Kuncová, joint project with ICT, supported by GA CR, grant No. 104/01/0461)

The influence of immobilization of living cells, *Sacharomyces cerevisiae* and *Pseudomonas sp. 2*, into silica matrix by sol-gel technique were followed with aim to use this technique for construction of optical biosensors. The optical method for on-line monitoring of fluorescence intensity of biogenic fluorophores of living cells immobilized in translucent carriers were developed and verified by measurements of different concentrations of alginate immobilized *Sacharomyces sp. 4*. [Refs. 7, 17, 33, 38, 39]

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)

The project is aimed at the development of novel enzyme-based fibre optic sensors for applications in biotechnological production processes to cover the lack of sensors suitable for *in situ* continuous monitoring of reactants under harsh reaction conditions. The project was started at the meeting held in ICPF AS CR in Prague in November 2002.

International co-operations

Instituto Superior Técnico, Lisbon, Portugal: Electrochemistry of transition metal complexes with azine ligands

Visitors

R. Gedye, Laurentian University, Sudbury, Canada

D. Agraval, Material Research Institute, Pennsylvania State University, USA

Y. Nikawa, Kokushikan University, Tokyo, Japonsko

Teaching

F. Kašánek: ICT, course "Bioengineering"

Publications

Original papers

1. Almeida F.M.T., Carvalho M.F.N.N., Galvao A.M., Čermák Jan, Blechta V., Pombeiro A.J.L., Shaw B.L.: Cationic Nickel(II) Complexes with Azine Diphosphines - Structural and Electrochemical Study. Inorg. Chim. Acta 338, 201-209 (2002).

2. Bříza T., Kvíčala J., Paleta O., Čermák Jan: Preparation of Bis(polyfluoroalkyl)cyclopentadienes, New Highly Fluorophilic Ligands for Fluorous Biphasic Catalysis. *Tetrahedron* 58(20), 3841-3846 (2002).
3. Chomát M., Berková D., Matějec V., Kašík I., Kuncová G., Gagniere H., Trouillet A., Bardin F.: Optical Detection of Toluene in Water by Using IGI Fibers. *Mater. Sci. Eng. C* 21(1-2), 211-215 (2002).
4. Chomát M., Berková D., Matějec V., Kašík I., Kuncová G., Hayer M.: Optical Detection of Toluene in Water Using an IGI Optical Fiber With a Short Sensing Region. *Sens. Actuators, B* 87(2), 258-267 (2002).
5. Církva V., Kaplánek R., Paleta O., Kodíček K.: Amphiphilic Perfluoroalkylated Derivatives of Aliphatic Triols: Hemocompatibility and Effect on Perfluorocarbon Emulsion. *Collect. Czech. Chem. Commun.* 67(10), 1436-1448 (2002).
6. Kuncová G., Hetflejš J., Szilva J., Šabata S.: Immobilization of Biomaterials into Organic-Inorganic Matrices. *Landbauforschung Volkenrode* 241, 41-46 (2002).
7. Kuncová G., Tříška J., Vrchotová N., Podrazký O.: The influence of Immobilization of *Pseudomonas* sp. 2 on Optical Detection of Polychlorinated Biphenyls. *Mater. Sci. Eng., C* 21(1-2), 195-201 (2002).
8. Kvíčala J., Bříza T., Paleta O., Auerová K., Čermák Jan: Synthesis, Fluorophilicities and Regioisomer Composition of Ferrocenes and Rhodium Complexes Based on Bis(polyfluoroalkylated) Cyclopentadienes. *Tetrahedron* 58(20), 3847-3854 (2002).
9. Kvíčala J., Bříza T., Paleta O., Čermák Jan: Synthesis of (Polyfluoroalkyl)cyclopentenes as Model Compounds for Fluorophilic Cyclopentadienes. *Collect. Czech. Chem. Commun.* 67(9), 1345-1358 (2002).
10. Murová I., Hájek M., Lovás M.: Využitie mikrovlnnej energie pri interakcii s anorganickými zlúčeninami a nerastnými surovinami. (Slov) Application of Microwave Energy to Inorganic Compounds and Raw Materials. *Chem. Listy* 96(4), 182-187 (2002).
11. Radoiu M., Hájek M.: Effect of Solvent, Catalyst Type and Catalyst Activation on the Microwave Transformation of 2-tert-Butylphenol. *J. Mol. Catal.* 186(1-2), 121-126 (2002).
12. Šabata S., Hetflejš J.: Hydrogenation of Low Molar Mass OH-Telechelic Polybutadienes Catalyzed by Homogeneous Ziegler Nickel Catalysts. *J. Appl. Polym. Sci.* 85(6), 1185-1193 (2002).
13. Kuncová G., Szilva J., Hetflejš J., Šabata S.: Catalysis in Organic Solvents with Lipase Immobilized by Sol-Gel Technique. *J. Sol-Gel Sci. Technol.* 26(1-3), 1183-1187 (2003).
14. Církva V., Duchek J., Paleta O.: Fluorinated Epoxides. 6. Chemoselectivity in the Preparation of 2-[(Heptafluoroisopropyl)methyl]oxirane from Iodoacetate and Iodohydrin Precursors. *J. Fluorine Chem.*, submitted.
15. Kaštánek F.: System of Decontamination of Wastes Containing PCBs. *J. Hazard. Mater.*, in press.
16. Kurfürstová J., Hájek M.: Microwave-Induced Catalytic Transformation of 2-tert-Butylphenol at Low Temperatures. *JMPEE*, in press.
17. Marseaut S., Debourg A., Dostálek P., Votruba J., Kuncová G.: Biosorbent of Heavy Metals with Silica Matrix. *Int. Biodeterior. Biodeg.*, in press.
18. Murová I., Hájek M., Lovás M.: Využitie mikrovlnnej energie pri chemickej úprave nerastných surovín. (Slov) Application of Microwave Energy in Chemical Modification of Minerals. *Chem. Listy*, in press.
19. Škvára F., Kaštánek F., Pavelková I., Šolcová O., Maléterová Y., Schneider P.: Solidification of waste steel foundry dust with Portland cement. *Journal of Hazardous Materials* B89, 67-81 (2002)

20. Kaštánek F., Páca J., Maléterová Y.: Biodegradation of Phenol at the Presence of Polyaromatic Hydrocarbons (PAH) in Soil. *Int. Biodeterior. Biodeg.*, submitted.

Chapters in books

21. Hájek M.: Microwave Catalysis in Organic Synthesis. In: *Microwaves in Organic Synthesis*, Chapter 10. (Loupy, A., Ed.), pp. 345-378, Wiley-VCH, Weinheim 2002.
22. Kaštánek F., Demnerová K., Macková M., Pazlarová J., Fava F., Macek T., Kučerová P., Matějů V., Sobotka M., Kaštánek P.: PCB-Approaches to Removal from the Environment. In: *Innovative Approaches to the On-Site Assessment and Remediation of Contaminated Sites*, NATO Sci. Ser., Vol. 15. (Reible, D. - Demnerova, K., Eds.), pp. 217-263, Kluwer Academic Press, London 2002.
23. Klán P., Církva V.: Microwave Photochemistry. In: *Microwaves in Organic Synthesis*, Chapter 14. (Loupy, A., Ed.), pp. 463-486, Wiley-VCH, Weinheim 2002.

Patents

24. Hájek M., Drahoš J.: Způsob vysoušení a desinfekce knih a papírových materiálů. (Czech) Method of Drying and Desinfection of Books and Paper Materials. Pat. No. PV2002-4272. Applied: 02.12.03.
25. Hájek M., Drahoš J.: Způsob a zařízení pro kontinuální výrobu vláken z přírodních surovin zvláště vulkanického původu. (Czech) Method and Equipment for Continuous Production of Fibers of Vulcanic Origin. Pat. No. PV2002-33428. Applied: 02.10.16.
26. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Vulcanic Origin. PCT/CZ00/00042/ (in press).

Conferences

27. Auerová K., Čermák Jan, Blechta V., Kvičala J.: 1-Hexyne Cyclotrimerization Catalyzed by Cyclopentadienyl Rhodium(I) Complexes. 13th International Symposium on Homogeneous Catalysis, Book of Abstracts, p. 310, Tarragona, Spain, 03-07 September 2002.
28. Církva V., Kurfürstová J., Hájek M.: Microwave Photochemistry of Substituted Phenols. XIXth IUPAC Symposium on Photochemistry, Book of Abstracts, p. 174-175, Budapest, Hungary, 14-19 July 2002.
29. Církva V., Paleta O.: Regioselectivity of Additions of Nucleophilic Radicals to Fluoroolefins. 37th ESF/EUCHEM Conference on Stereochemistry, Conference Report (*Chimia* 56, 432-438, 2002), p. 1, Bürgenstock, Switzerland, 13-19 April 2002.
30. Dostálek P., Čepička J., Fiala J., Prajzlerová M., Kuncová G.: Immobilization of Brewing Yeast Cells by Sol-Gel Technique. 4th Technical Meeting EBC Brewing Science Group, Book of Abstracts, p. 17, Oporto, Portugal, 04-06 September 2002.
31. Hájek M.: Microwave Catalysis in Organic Synthesis. International Symposium on Microwave Science and its Application to Related Fields, Book of Abstracts, p. 86, Nara, Japan, 21-23 November 2002.
32. Hájek M.: How to Make Bohemian Glass in Microwave Oven. International Symposium on Microwave Science and Its Application to Related Fields, Book of Abstracts, p. 1, Nara, Japan, 21-23 November 2002.

33. Jurčová I., Kuncová G., Burkhard J.: Determination of Biomass Concentration on Inorganic Carrier. X International BRG Workshop on Bioencapsulation, Book of Abstracts, p. 1-4, Praha, Czech Republic, 26-28 April 2002.
34. Kaštánek F.: New Technologies for Decontamination of Wastes Contaminated by PCBs and Dioxines. Environmental Opportunities in the Czech Republic, Book of Abstracts, Boston, Newark, USA, 06-10 May 2002.
35. Klán P., Literák J., Církva V., Hájek M.: Microwave Photochemistry. XIXth IUPAC Symposium on Photochemistry, Book of Abstracts, p. 70-71, Budapest, Hungary, 14-19 July 2002.
36. Kuncová G., Hetflejš J.: Inorganic and Organic/Inorganic Polymers for Entrapment of Biomaterials. Inventory of Polymers and Materials for the Encapsulation of Biocatalyst, Book of Abstracts, Liege, Belgium, 29-30 November 2002.
37. Montaňés A., Hetflejš J., Šabata S., Kuncová G.: Immobilization of Lipase on Mesoporous Silica Carrier. X International BRG Workshop on Bioencapsulation, Book of Abstracts, p. 148-151, Praha, Czech Republic, 26-28 April 2002.
38. Podrazký O., Kuncová G.: Monitoring of Immobilised Cells by 2-D Fluorescence Spectroscopy. 6th European Conference on Optical Chemical Sensors and Biosensors EUROPT(R)ODE VI, Book of Abstracts, p. 253, Manchester, Great Britain, 07-10 April 2002.
39. Prajzlerová M., Kuncová G., Dostálek P.: Immobilization of Brewing Yeast Cells by Sol-Gel Technique. X International BRG Workshop on Bioencapsulation, Book of Abstracts, p. 119-122, Praha, Czech Republic, 26-28 April 2002.
40. Smrček J., Hájek M., Vacek K., Vtípil S.: Využití infravize v teplotních profilech skloviny. (Czech) Application of Infravision in Temperature Profiles of Glass Melts. 11. Česká konference o skle, Sborník přednášek, p. 1, Praha, 11 April 2002.
41. Storch J., Čermák Jan, Včelák J., Czakoová M., Vojtíšek P.: Vinyl-Amide Palladium Complexes with Ene-Hydrazone Coordinated Diphosphinoazines. XXth International Conference on Organometallic Chemistry, Book of Abstracts, p. 269, Corfu, Greece, 07-12 July 2002.

Department of Reaction Engineering in Gas Phase

Head: M. Punčochář
Deputy: V. Ždímal

Research groups

Aerosol Laboratory
Group of Hydrodynamics and Chemistry of Incineration
Laboratory of Gas-Solid Systems, Emissions, and Waste Control
Laser Chemistry Group

Aerosol Laboratory

Research staff: J. Smolík, L. Džumbová, J. Kugler, V.V. Levdansky, P. Moravec,
J. Schwarz, I. Ševčíková, V. Ždímal
Part time: M. Barták
PhD student: D. Brus

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

Reduction of heavy metal emissions from fluidised bed coal combustion using sorbents
(J. Schwarz, supported by GA CR, grant No. 104/00/1297)

The project represents both experimental and theoretical effort aimed at solving important relationships in the complex processes of combustion, formation of particulate emissions, and behaviour of metal pollutants within a fluidised bed and in flue gas cleaning units. The experimental part is focused on interaction of mineral sorbents with metallic species emitted from the fluidised bed combustion of coal. Theoretical part uses thermodynamic approach to predict distribution of trace elements into different emission streams. [Refs. 9, 13, 14, 30, 32, 35]

Subgrid scale investigations of factors determining the occurrence of ozone and fine particles

(J. Smolík, supported by EC, grant No. EVK2-CT-1999-00052 SUB-AERO)

Objective of the project is the understanding of the formation, accumulation, fate, and effects of ozone, other photochemical oxidants and fine particulate matter in subgrid ("local") scale in the Mediterranean area. This is accomplished by incorporating state-of-the-art field measurements combined with the state-of-the-art analysis/mesoscale-subgrid modelling tools, which improve quantification of the relationships between emission source activity and ambient air quality for photochemical pollutants and fine particles. [Refs. 7, 10-12, 16-18, 33-35]

Characterization of urban air quality – indoor/outdoor particulate matter chemical characteristics and source-to-inhaled dose relationships

(J. Smolík, supported by EC, grant No. EVK4-CT-00018 URBAN-AEROSOL)

The project aims: (i) to characterize chemically the particulate matter associated with actual human exposure in selected residential European areas, (ii) to provide an integrated European exposure assessment database for urban PM characterization through indoor/outdoor monitoring and modelling, (iii) to study and evaluate the mechanisms controlling the indoor/outdoor relationships of PM by taking into account infiltration, meteorological conditions, indoor sources of PM, physical and chemical processes indoors, and the composition/size distribution of indoor generated particulate matter, by using mechanistically based models, and (iv) to link human exposure to particulate matter indoor with physiologically based mechanistic dosimetry models. [Refs. 15, 29, 31]

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.

Composite nanoparticle synthesis by CVD method in a hot-wall tube flow reactor

(P. Moravec, supported by GA CR, grant No. 104/02/1079)

The project involves an experimental study of both monocomponent and multicomponent nanoparticle synthesis by CVD method in an externally heated tube flow reactor. The synthesised particles should be metal oxide particles as ZrO_2 , Fe_2O_3 , Ta_2O_3 or V_2O_5 , metallic particles as Fe, Cu or Ni and mixed and/or composite multicomponent particles as ZrO_2/SiO_2 ,

V₂O₅/SiO₂, Cu/SiO₂, Fe/TiO₂. Particle morphology, crystallinity and chemical composition are examined by SEM, TEM, SAED, XRD and EDS. [Refs. 8, 26-28]

Aerosol particle growth in presence of foreign gas and problem of foreign molecule trapping

(V.V. Levdansky, supported by GA ASCR, grant No. IAA4072205)

The aim of the proposed project is to perform a theoretical study of impurity molecule trapping by growing aerosol particles during condensation process. Mathematical modelling of the impurity molecule concentration in aerosol particles and determination of the probability (coefficient) of the impurity molecule trapping is to be done for two cases: 1) impurity molecules are either present in the volume considered or enter it from the surrounding medium, 2) impurity molecules appear in the volume as a result of a chemical reaction in the gas phase. The methods for removing impurity molecules from the gas phase will be elaborated, based on the above mentioned trapping. The influence of external fields (e.g., resonance laser radiation) on this kind of trapping will be studied as well. It is also assumed to study the effect of foreign (buffer) gas on the deposition rate in aerosol systems. [Refs. 2, 3, 19-25]

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 vapors. 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. 25, 36, 37]

International co-operations

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

University of Helsinki, Helsinki, Finland: Condensation processes as a part of gas-to-particle conversion

Finnish Meteorological Institute, Helsinki, Finland: Application of cascade impactors for aerosol studies

Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece: Urban aerosols

Norwegian Institute for Air Research, Kjeller, Norway: Formation of ozone and fine particles in the Mediterranean area

University of Essex, Colchester, Great Britain: Sampling of fine atmospheric particles

Institute for Systems, Informatics and Safety, JRC-Ispra, Italy: Modelling of fine particle formation

Technical University of Crete, Chania, Greece: Aerosols in the environment

Fraunhofer Institute FhITEM, Hannover, Germany: Indoor/outdoor aerosols

Tampere University of Technology, Tampere, Finland: Synthesis and characterisation of nanosized metal/ceramic particles
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

Visitors

H. Keskinen, Institute of Physics, Tampere University of Technology, Tampere, Finland
Ü. Kikas, Institute of Environmental Physics, University of Tartu, Tartu, Estonia
S.K. Zaripov, Chebotarev Institute of Mathematics and Mechanics, Kazan State University, Kazan, Russia

Publications

Original papers

1. Bakanov S.P., Ždímal V., Zaripov Sh.Kh., Smolík J.: Dvizhenie aerosol'noi kapli v termodiffuzionnoi kamere. (Russ) Motion of an Aerosol Particle in a Thermal Diffusion Cloud Chamber. *Prikl. Mat. Mekhan.* 66(1), 95-101 (2002).
2. Levdansky V.V., Smolík J., Moravec P., Ždímal V.: Chemical Deposition on Aerosol Particles. *J. Eng. Phys. Therm.* (Translated from *Inzh.-Fiz. Zh.* 75(3), 118-121, 2002) 75(3), 670-675 (2002).
3. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Growth and Evaporation of Aerosol Particles in the Presence of Adsorbable Gases. *Int. J. Heat Mass Transfer* 45(18), 3831-3837 (2002).
4. Maenhaut W., Schwarz J., Cafmeyer J., Annegarn H.J.: Study of Elemental Mass Distributions at Skukuza, South Afrika, during the SAFARI 2000 Dry Season Campaign. *Nucl. Instrum. Methods Phys. Res., Sect B* 189, 254-258 (2002).
5. Maenhaut W., Schwarz J., Cafmeyer J., Chi X.: Aerosol Chemical Mass Closure during the EUROTRAC-2 AEROSOL Intercomparison 2000. *Nucl. Instrum. Methods Phys. Res., Sect B* 186, 233-237 (2002).
6. Petrova T.S., Semkov K.A., Moravec P.: Determination of the Characteristic Packing Size in the Mathematical Model for Liquid Phase Spreading in Packed-Bed Columns with Deflecting Rings. *Bulgar. Chem. Commun.* 34(1), 82-98 (2002).
7. Bardouki H., Liakakou H., Economou C., Sciare J., Smolík J., Ždímal V., Eleftheriadis K., Lazaridis M., Dye C., Mihalopoulos N.: Chemical Composition of Size Resolved Atmospheric Aerosols in the Eastern Mediterranean during Summer and Winter. *Atmos. Environ.*, in press.
8. Moravec P., Smolík J., Levdansky V.V.: Preparation of Al₂O₃-SiO₂ Fine Particles by CVD Method in Tube Flow Reactor. *Powder Technol.*, submitted.
9. Sýkorová I., Smolík J., Pešek J., Machovič V.: Composition and Mode of Occurrence of the Mineral Constituents in Brown Coal and Their Behaviour at Fluidized Bed Combustion. *Acta Montana Series AB*, in press.

10. Večeřa Z., Mikuška P., Smolík J., Eleftheriadis K., Bryant C., Colbeck I., Lazaridis M.: Shipboard Measurements of Ozone, Nitrogen Dioxide, Nitrous and Nitric Acids, and Sulphur Dioxide in the Eastern Mediterranean. *J. Geophys. Res.*, submitted.

Chapters in books

11. Smolík J., Ždímal V., Lazaridis M., Schwarz J., Havránek V., Eleftheriadis K., Colbeck I., Mihalopoulos N., Nyeki S., Housiadas C.: Size Resolved Mass Concentration and Chemical Composition of Atmospheric Aerosols over the Eastern Mediterranean Area. In: *Measurements of Particulate Matter: Status Report 2002*. (Kahnert, M., Ed.), pp. 26-51, Norwegian Institute for Air Research, Kjeller 2002.
12. Lazaridis M., Spiridaki A., Solberg S., Svendby T., Svenby T., Kallos G., Flatoy F., Housiadas C., Smolík J., Colbeck I., Eleftheriadis K.: Modelling of Aerosol Processes in the Mediterranean Area. In: *NATO Conference on Regional Atmospheric Modelling*. (Eng.), Kluwer Academic Press, in press.

Conferences

13. Havránek V., Voseček V., Smolík J., Schwarz J., Ždímal V.: Analysis of Aerosol Samples by Energetic Ion Beam. *Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56*, pp. 47-51, Prague, Czech Republic, 23-26 May 2002.
14. Kučera J., Smolík J., Schwarz J., Havránek V.: INAA and PIXE of Combustion Aerosols. 2002 Winter Meeting American Nuclear Society, *Transactions*, p. 456-457, Washington, D.C., USA, 17-21 November 2002.
15. Lazaridis M., Asimakopoulos D.N., Braniš M., Colbeck I., Drossinos I., Dye C., Eleftheriadis K., Flocas H., Helmis C., Hollander W., Smolík J., Ždímal V.: Characterisation of Urban Air Quality and Indoor/Outdoor Particulate Matter Chemical Characteristics. *Sixth International Aerosol Conference, Abstracts*, p. 1227-1228, Taipei, Taiwan, 09-13 September 2002.
16. Lazaridis M., Colbeck I., Drossinos I., Eleftheriadis K., Havránek V., Housiadas C., Kallos G., Mihalopoulos N., Smolík J., Večeřa Z., Ždímal V., Solberg S.: Characterization of Physical and Chemical Factors Determining the Occurrence of Ozone and Fine Particles. *7th Scientific Conference of the International Global Atmospheric Chemistry Project (IGAC), Book of Abstracts*, p. 98, Heraklion, Crete, Greece, 18-25 September 2002.
17. Lazaridis M., Kallos G., Spiridaki A., Solberg S., Svendby T., Drissinos I., Housiadas C., Smolík J., Colbeck I., Eleftheriadis K., Gekas V.: Modelling of Combined Aerosol and Photooxidant Dynamics in the Mediterranean Area. *International Conference Protection and Restoration of the Environment VI, Volume*, p. 1051-1056, Skiathos, Greece, 01-05 July 2002.
18. Lazaridis M., Kallos G., Spiridaki A., Solberg S., Svendby T., Flatøy F., Drossinos I., Housiadas C., Smolík J., Colbeck I., Eleftheriadis K., Ždímal V.: Modelling of Combined Aerosol and Photooxidant Processes in the Mediterranean Area. *Sixth International Aerosol Conference, Abstracts*, p. 1241-1242, Taipei, Taiwan, 09-13 September 2002.
19. Levčanský V.V., Smolík J.: Internal Problems of Thin Film Deposition from Gas Phase. *12th International Conference on Thin Films, Book of Abstracts*, p. TF1.6.0, Bratislava, Slovakia, 15-20 September 2002.

20. Levdansky V.V., Smolík J., Moravec P.: Impurity Molecule Trapping in Deposition from Gas Phase. 9th Joint Vacuum Conference JVC-9, Book of Abstracts, pp. 82-83, Schlos Seggau, Austria, 16-20 June 2002.
21. Levdansky V.V., Smolík J., Moravec P.: Effect of Laser Radiation on Composition and Growth Rate of Aerosol Particles. E-MRS Spring Meeting 2002, Book of Abstracts, p. D-14, Strasbourg, France, 18-21 June 2002.
22. Levdansky V.V., Smolík J., Moravec P.: Joint Effect of Mass Transfer and Surface Processes in Growth (Evaporation) of Small Drops. 6th International Aerosol Conference., Abstracts, pp. 493-494, Taipei,, Taiwan, 09-13 September 2002.
23. Levdansky V.V., Smolík J., Moravec P.: Joint Effect of Diffusion and Kinetic Resistances in Growth of Small Aerosol Particles. VI International School-Seminar Nonequilibrium Processes and Their Applications, Contributed Papers, p. 19-22, Minsk, Belarus, 31 August - 05 September 2002.
24. Levdansky V.V., Smolík J., Moravec P., Ždímal V.: Vliyanie adsorbiruyushchikhsya gazov na rost i isparenie malykh aerazol'nykh chastits. (Russ) Effect of Adsorbable Gases on Growth and Evaporation of Small Aerosol Particles. Trudy Tret'ei Rossiiskoi Natsionalnoi Konferentsii po Teploobmenu, Tom 4, p. 296-299, Moskva, Russia, 21-25 October 2002.
25. Levdansky V.V., Smolík J., Ždímal V., Moravec P.: Kinetics of Chemical Deposition on Aerosol Particles. 6th International Aerosol Conference, Poster last minute, p. 1309-1310, Taipei, Taiwan, 09-13 September 2002.
26. Moravec P., Smolík J., Levdansky V.V.: Synthesis of TiO₂-SiO₂ Fine Particles by CVD Method in a Single Tube Flow Reactor. Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56, pp. 119-122, Prague, Czech Republic, 23-26 May 2002.
27. Moravec P., Smolík J., Levdansky V.V., Keskinen H.: Synthesis of Heterostructure Fine Particles by CVD Method in a Tube Flow Reactor. NANO'02 National Conference, Book of Abstracts, p. 35, Brno, Czech Republic, 19-21 November 2002.
28. Moravec P., Smolík J., Levdansky V.V., Keskinen H.: CVD Synthesis of Multicomponent Nanosized Particles in an Externally Heated Tube Flow Reactor. Symposium Nano-Structured Materials – Fundamentals and Applications, Book of Abstracts, p. 1, Vienna, Austria, 27-28 November 2002.
29. Smolík J., Ždímal V., Schwarz J., Holländer W., Lazaridis M.: Time and Size Resolved Indoor/Outdoor Particles in an Empty Room. Sixth International Aerosol Conference, Abstracts, p. 1089-1090, Taipei, Taiwan, 09-13 September 2002.
30. Smolík J., Džumbová L., Schwarz J., Leitner J., Sýkorová I.: Thermodynamic Analysis of Trace Elements Partitioning in AFBC Combustion of Lignite. Sixth International Aerosol Conference, Abstracts, p. 191-192, Taipei, Taiwan, 09-13 September 2002.
31. Smolík J., Holländer W., Ždímal V., Schwarz J., Lazaridis M.: Temporal Variation of Indoor Aerosol in an Empty Room without Internal Particle Sources. Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56, pp.138-141, Prague, Czech Republic, 23-26 May 2002.
32. Smolík J., Schwarz J., Džumbová L., Kugler J., Veselý V., Sýkorová I., Kučera J., Havránek V., Leitner V.: An Equilibrium Analysis of Behavior of Trace Elements during Fluidized Bed Combustion of Lignite. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 274, Prague, Czech Republic, 25-29 August 2002.
33. Smolík J., Ždímal V., Eleftheriadis K., Havránek V., Mihalopoulos N., Schwarz J., Colbeck I., Lazaridis M.: Size Resolved Chemical Composition of Atmospheric Aerosols

- Collected in Winter over the Eastern Mediterranean Area. Sixth International Aerosol Conference, Abstracts, p. 301-302, Taipei, Taiwan, 09-13 September 2002.
34. Smolík J., Ždímal V., Eleftheriadis K., Havránek V., Mihalopoulos N., Schwarz J., Colbeck I., Lazaridis M.: Characterization of Size-Fractionated Atmospheric Aerosol Collected in the Eastern Mediterranean Region. Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56, pp. 142-145, Prague, Czech Republic, 23-26 May 2002.
 35. Wagner Z., Ždímal V., Smolík J.: Application of Gnostic Theory to Analysis of Particle Size Distribution. Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56, pp. 164-168, Prague, Czech Republic, 23-26 May 2002.
 36. Ždímal V., Brus D., Matas J.: Homogeneous Nucleation Rates in Supersaturated Vapor of n-Propanol: Raw Results. Sixth International Aerosol Conference, Poster last minute, p. 1307-1308, Taipei, Taiwan, 09-13 September 2002.
 37. Ždímal V., Brus D., Matas J.: Homogeneous Nucleation Rates of n-Propanol in a Static Diffusion Chamber: First Results. Czech-Finnish Aerosol Symposium, Report Series in Aerosol Science, No 56, pp. 175-180, Prague, Czech Republic, 23-26 May 2002.

Group of Hydrodynamics and Chemistry of Incineration

Research staff: M. Punčochář, E. Fišerová, V. Gruber, V. Pekárek, V. Tydlitát, V. Veselý,
L. Vlková
Technical staff: J. Chour, J. Ullrich
PhD student: S. Chytil

Fields of research

- Persistent organic pollutants
- Gas-solid reactions
- Fluidized bed combustion

Applied research

- Dechlorination of persistent organic pollutants
- Recovery of precious metals

Research projects

Power combustion of wastes and biomass

(M. Punčochář, supported by GA CR, grant No. 104/97/S002)

The mechanism of dioxins emission suppression due to sulphur additives was studied. Particularly the effect of green vitriol, which is industrial waste from the production of titanium dioxide, was found as very promising. We compared also the effect of sulphates as additives with pure sulphur and we found twice as strong effect for the sulphates. Further, the study of reaction time revealed that PCDD and PCDF arise by two – different fast-reactions. The fastest is formation of PCDD by Stieglitz mechanism from destructed carbon or via direct condensation from phenols. The prevailing mechanism for PCDF formation are slower reactions based on Ullman reactions and condensation of hydroxybiphenyls. [Refs. 3, 10, 14]

Deactivation of fly ash as a catalyst in de novo synthetic reactions producing persistent organic pollutants (POP)

(V. Pekárek, supported by GA ASCR, grant No. A4072206)

The basic study of suppression of so-called de novo synthetic reactions forming highly toxic persistent organic pollutants was done. The effects of some sulphur containing compounds added into the gas phase as well as of some complexing or chemical agents added to the reaction matrix are under study. [Refs. 2, 6, 7, 10, 11, 22, 24]

Continuous pilot plant equipment for detoxification of persistent organic compounds (PCBs, PCDD/Fs) in fly ash, carbon absorbers and soils

(V. Pekárek, supported by GA ASCR, grant No.S4072108)

The main results of the grant, focussed on application of the basic results to praxis, verified that the constructed semi-continual detoxification apparatus for ca. 50 kg loading is more efficient as compared with laboratory experiments. It was proved that different polychlorinated toxic substances were totally detoxified more than from 99%. The samples from the floor of the highly contaminated object from Spolana Neratovice, which contained complex mixture of dioxins and dioxins-like compounds, were detoxified from 99.99%. [Ref. 20]

The study of the POPs formation during combustion of used oils in commercial low-output boilers with the aim to reduce their formation

(V. Pekárek, V. Tydlitát, supported by GA CR, grant No. 101/01/0830)

The oil combustion on low power boilers with evaporation or burner heating construction was studied in the co-operation with National Reference Laboratory for POP compounds in Frýdek-Místek. Two types of used oils were combusted (No.1 - a mixture of oils from Diesel engines and Diesel gear oils coming from a large repair shop. No.2 - a mixture of motor oils of the viscosity 15W40 from ÖMV used in Diesel trucks). A surprising statement follows from our measurements: the limit $0,1 \text{ ng TEQ}\cdot\text{m}^{-3}$ for PCDD/F was only moderately exceeded ($0,295 \text{ ng TEQ}\cdot\text{m}^{-3}$ for the first oil and $0,136 \text{ ng TEQ}\cdot\text{m}^{-3}$ for the second one). [Refs. 4, 5, 27]

International co-operations

Vrije Universiteit Brussels, Belgium: Formation of POPs

Forschungszentrum Karlsruhe, Institut für Technische Chemie, Karlsruhe, Germany: Dioxin chemistry

Publications

Original papers

1. Drahoš J., Punčochář M.: Comments on Application of the Fractional Brownian Motion in an Airlift Reactor. *Chem. Eng. Sci.* 57(10), 1831-1832 (2002).
2. Grabic R., Pekárek V., Fišerová E., Ullrich J., Karban J., Crhová Š., Tomšej T.: Study of the Effect of Matrix on Formation of PCDD, PCDF, PCB and PCBZ by De novo Synthetic Reactions under Model Laboratory Conditions. *Organohalogen Compd.* 56, 205-208 (2002).
3. Grabic R., Pekárek V., Ullrich J., Punčochář M., Fišerová E., Karban J., Šebestová M.: Effect of Reaction Time on PCDD and PCDF Formation by De novo Synthetic Reactions under Oxygen Deficient and Rich Atmosphere. *Chemosphere* 49(7), 691-696 (2002).
4. Tydlitát V., Pekárek V., Janota J.: Emise toxických složek při spalování motorových olejů. (Czech) Emissions of Toxic Components from Waste Engine Oils Combustion. *Odpady* 12(1), 16-18 (2002).
5. Tydlitát V., Pekárek V., Janota J.: Toxické látky ve spalinách odpadních olejů z odpařovacího kotle 29 kW. (Czech) Toxic substances in flue gases from 29 kW Pan Evaporation Boiler with Waste Oil Fuel. *Ochrana ovzduší* 14(3-4), 33-37 (2002).
6. Bureš M., Pekárek V., Karban J., Fišerová E.: Dehalogenation Properties of Municipal Fly Ash. II. Comparison of Dehalogenation Pathway of Fly Ash and Model Fly Ash with Thermodynamic Calculations. *Environ. Sci. Pollut. Res.*, in press.
7. Bureš M., Pekárek V., Wolf G., Punčochář M.: Thermochemical Quantities of Polychlorinated Biphenyls in Ideal Gas State. *Environ. Sci. Technol.*, submitted.
8. Hartman M., Trnka O., Svoboda K., Veselý V.: Thermal Dissociation and H₂S Reactivity of Czech Limestones. *Chem. Pap.*, in press.
9. Jochová M., Punčochář M., Horáček J., Štamberg K., Vopálka D.: Removal of Heavy Metals from Water by Lignite-Based Sorbents. *Fuel*, submitted.
10. Pekárek V., Grabic R., Punčochář M., Ullrich J., Fišerová E., Bureš M.: Effect of Sulphur Dioxide, Hydrogen Peroxide, Sulphuric Acid and Their Mixtures on the De-novo Synthesis of PCDD and PCDF in the N₂ + 10% O₂ Atmosphere Under Model Laboratory Conditions. *Chemosphere*, in press.
11. Pekárek V., Karban J., Fišerová E., Bureš M., Pacáková V., Večerníková E.: Dehalogenation Properties of the Municipal Waste Incineration Fly Ash. I. General Principles. *Environ. Sci. Pollut. Res.*, in press.
12. Pekárek V., Punčochář M.: Výsledky základního a aplikovaného výzkumu v oblasti chemie polychlorovaných bifenyly (PCB), dibenzo-p-dioxinů (PCDD), dibenzofuranů (PCDF) a chlorbenzenů (PCBz) v Ústavu chemických procesů AV ČR. (Czech) Results of Basic and Applied Research in the Field of the Chemistry of Polychlorinated Biphenyls (PCB), Dibenzo-p-dioxines (PCDD), Dibenzofurans and Chlorobenzenes (PCBz) in the Institute of Chemical Process Fundamentals of the Academy of Sciences of the Czech Republic. *Ochrana ovzduší*, in press.
13. Punčochář M., Drahoš J.: Entropy of Fluidized Bed – a Measure of Particle Mixing. *Chem. Eng. Sci.*, submitted.

14. Punčochář M., Veselý V.: Dioxinový program na poloprovozním fluidním ohništi ÚChP AV ČR. (Czech) Dioxin Program on the Pilot-Plant Fluidized Bed of Institute of Chemical Process Fundamentals ASCR. Ochrana ovzduší, submitted.

Review papers

15. Hartman M., Svoboda K., Trnka O., Veselý V.: Reakce vápenatých a hořečnatých materiálů při vysokoteplotním odsiřování spalin a energetického plynu. (Czech) Reactions of Calcareous and Magnesian Compounds in the Desulfurization of Flue and Coal Gas at High Temperature. Chem. Listy 96(10), 777-783 (2002).
16. Hartman M., Svoboda K., Veselý V., Trnka O., Chour J.: Nakládání s čistírenskými kaly. (Czech) Sewage Sludge Processing. Chem. Listy, in press.
17. Hartman M., Trnka O., Svoboda K., Veselý V.: Aglomerace částic a defluidizační jevy ve fluidní vrstvě. (Czech) Agglomeration of Particles and Defluidization Phenomena in the Fluid bed. Chem. Listy, submitted.

Chapters in books

18. Drahoš J., Punčochář M.: Fraktály a chaos: další z vědeckých revolucí 20. století? (Czech) Fractals and Chaos: Another 20th Century Scientific Revolution? In: Myšlenky na zlomu tisíciletí. (Czech). Thoughts for the New Millenium (Mizerová, A. - Sedlák, J. - Dub, P., Eds.), pp. 255-277, VUTIUM, Brno 2002.
19. Punčochář M.: Nakládání s nebezpečnými odpady. (Czech) Treatment of Hazardous Wastes. In: K udržitelnému rozvoji České republiky: vytváření podmínek. (Czech). Contribution to Sustainable Development of the CR (Moldan, B. - Hák, T. - Kolářová, H., Eds.), pp. 313-336, Univerzita Karlova, Frýdek-Místek 2002.

Patents

20. Pekárek V., Hapala P., Fišerová E.: Způsob dehalogenace halogenovaných aromatických sloučenin. (Czech) Method of Aromatic Halogenated Compounds Dehalogenation. Pat. No. PV 2001-4370. Applied: 01.12.05.
21. Veselý V., Trnka O., Hartman M.: Způsob řízení a identifikace režimu fluidní vrstvy zrnitého materiálu. (Czech) Control and Identification of a Regime of the Fluidized Bed. Pat. No. PV 314-99. Applied: 01.04.01.

Conferences

22. Bureš M., Pekárek V.: Dehalogenace polychlorovaných fenolů. (Czech) Dehalogenation of Polychlorinated Phenols. Kalorimetrický seminář 2002, Sborník příspěvků, p. 115-118, Seč u Chrudimi, Czech Republic, 27-31 May 2002.
23. Pekárek V., Buekens A., Stieglitz L., Grabic R.: Reaction of Metallic Chloride with Copper as Probable Reason for PCDD/F, PCB and PCBz Formation in Iron Metallurgical Plant. 13th International F.W. Karasek Conference, Book of Abstracts, p. 1, Kiawah Island Resort, USA, 05-08 May 2002.
24. Pekárek V., Grabic R.: The Results of Basic Research in the Field of Dehalogenation and De novo Synthesis of PCDD/F, PCB and PCBz. VI Konferencja Naukowa Dioksyny w Przemysle i Środowisku., p. 14-18, Kraków-Tomaszowice, Poland, 26-27 September 2002.

25. Punčochář M., Veselý V.: Application of Reactive Barrier for Decontamination of Groundwater in Industrial Plant. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 157, Tatranské Matliare, Slovakia, 27-31 May 2002.
26. Smolík J., Schwarz J., Džumbová L., Kugler J., Veselý V., Sýkorová I., Kučera J., Havránek V., Leitner V.: An Equilibrium Analysis of Behavior of Trace Elements during Fluidized Bed Combustion of Lignite. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 1, p. 274, Prague, Czech Republic, 25-29 August 2002.
27. Tydlitát V., Janota J., Pekárek V., Punčochář M.: Emissions of Toxic Components from Firing of Used Oils in a 102 kW Burner Boiler. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 5, p. 190, Prague, Czech Republic, 25-29 August 2002.
28. Veselý V., Punčochář M.: Using of Zero Valent Iron for Groundwater Decontamination. 29th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 12, Tatranské Matliare, Slovakia, 27-31 May 2002.

Laboratory of Gas-Solid Systems, Emissions, and Waste Control

Research staff: K. Svoboda, M. Hartman, O. Trnka

Technical staff: M. Pohořelý

Fields of research

- Gas-solid reactions
- Gas-solid reactors and operations
- Fluidized bed combustion
- Gaseous and particulate emissions from combustion and industrial processes
- Solid waste treatment and co-combustion

Research projects

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. 6, 10]

Agglomeration in fluidized-bed reactors

(M. Hartman, supported by GA CR, grant No. 203/02/0002)

The study is aimed at resolving the troublesome problems in fluidized-bed processes at conditions where particles are sticky and agglomeration tends to occur. The subject of research is the capability of a fluidized bed to handle particulate solids becoming sticky/wet by the presence of liquids or during chemical reactions taking place within the bed. [Refs. 9, 11]

Pressurized fluidized bed combustion of coal, emissions of nitrogen oxides and effect of biomass addition to the fuel on emissions and behaviour of the pressurized fluidized bed under combustion conditions

(K. Svoboda, supported by GA ASCR, grant No. A4072801)

The project in the field of Clean Coal Technology and biomass-co-combustion is concentrated on experimental investigation and modelling of pressurized bed combustion of coal and biomass-coal blends. Target of the research work: emissions (NO_x , N_2O , CO , SO_2), maximum particle temperature and agglomeration of coal/biomass-ash particles. [Refs. 2, 4, 7, 8, 13, 15, 16]

Evaluation of dynamic states of gas fluidized suspensions via pressure fluctuations

(O. Trnka, supported by GA ASCR, grant No. A4072001)

Research is oriented on developing new tools for the on-line diagnostics of flow regimes in fluidized beds. Pressure fluctuations within the beds are measured and subjected to detailed analysis. Novel and rigorous computational procedures are developed for the evaluation of pressure fluctuation time series. [Refs. 11]

International co-operations

University College London, London, Great Britain: High temperature fluidization

University of Connecticut, Storrs, USA: Desulfurization of Gases

Delft University of Technology, Delft, the Netherlands: Circulating fluidized beds

Technical University Cottbus, Germany: Pressurized fluidized bed combustion

Institute of Physical Chemistry, PAS, Warsaw, Poland: Fluidized bed operations

Institute for Energy, Joint Research Centre, Petten, the Netherlands: Pressurized fluidized bed combustion/gasification technologies

Visits abroad

K. Svoboda: Institute for Energy, Joint Research Centre of European Commission, Petten, the Netherlands (3 months)

Visitors

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

Teaching

M. Hartman: ICT, postgraduate course "Multiphase reactors"

K. Svoboda: ICT, course "Environmental engineering"

Publications

Original papers

1. Hartman M., Svoboda K., Trnka O.: Comments on "Design of Entrained-Flow and Moving-, Packed-, and Fluidized-Bed Sorption Systems: Grain-Model Kinetics for Hot Coal-Gas Desulfurization with Limestone". *Ind. Eng. Chem. Res.* 41, 1914-1915 (2002).
2. Hartman M., Svoboda K., Trnka O., Čermák Ji.: Reaction between Hydrogen Sulfide and Limestone Calcines. *Ind. Eng. Chem. Res.* 41(10), 2392-2398 (2002).
3. Hartman M., Trnka O.: Comments on "Proposal for a Regenerative High-Temperature Process for Coal Gas Cleanup with Calcined Limestone". *Ind. Eng. Chem. Res.* 41(24), 6207-6208 (2002).
4. Svoboda K., Hartman M., Čermák Ji.: Effect of Pressure and Temperature on Coal Behaviour in PFBC/G. *Acta Montana, Ser. B*, 126(12), 63/79 (2002).
5. Hartman M., Trnka O., Svoboda K.: Textural Changes in Solids due to the Chemical Reactions. *AIChE J.*, in press.
6. Hartman M., Trnka O., Svoboda K., Veselý V.: Thermal Dissociation and H₂S Reactivity of Czech Limestones. *Chem. Pap.*, in press.
7. Svoboda K., Pohořelý M.: Influence of Operating Conditions and Coal Properties on NO_x and N₂O Emissions in Pressurized Fluidized Bed Combustion of Subbituminous Coals. *Fuel*, submitted.
8. Svoboda K., Pohořelý M., Hartman M.: Effects of Operating Conditions on the NO_x, N₂O and CO Emissions in PFB Co-combustion of Coal and Wood. *Energy Fuels*, in press.

Review papers

9. Hartman M., Svoboda K., Trnka O., Veselý V.: Reakce vápenatých a hořečnatých materiálů při vysokoteplotním odsiřování spalin a energetického plynu. (Czech) Reactions of Calcareous and Magnesian Compounds in the Desulfurization of Flue and Coal Gas at High Temperature. *Chem. Listy* 96(10), 777-783 (2002).
10. Hartman M., Svoboda K., Veselý V., Trnka O., Chour J.: Nakládání s čistírenskými kaly. (Czech) Sewage Sludge Processing. *Chem. Listy*, in press.
11. Hartman M., Trnka O., Svoboda K., Veselý V.: Aglomerace částic a defluidizační jevy ve fluidní vrstvě. (Czech) Agglomeration of Particles and Defluidization Phenomena in the Fluid Bed. *Chem. Listy*, submitted.
12. Svoboda K., Čermák Ji., Trnka O., Hartman M.: Vysokoteplotní palivové články, vhodná paliva a možnosti jejich využití. (Czech) High Temperature Fuel Cells, Their Status, Fuels and Applications. *Chem. Listy*, in press.

Patents

13. Svoboda K., Čermák Ji., Hartman M., Bařalík J., Gubčo V.: Způsob energetického využití tuhých paliv s tlakovým zplyňováním a paro-plynovým cyklem a zařízení k jeho provádění. (Czech) Method and Apparatus for Solid Fuel Pressurized Gasification with Combined Cycle Power Generation. Pat. No. 290861. Applied: 01.03.21, Patented: 02.09.03.

Conferences

14. Čermák Ji., Svoboda K., Pohořelý M.: Release and Partition of Selected Alkali Metals and Heavy Metals in Pressurized Substoichiometric Combustion of Coals. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 5, p. 191, Prague, Czech Republic, 25-29 August 2002.
15. Svoboda K., Čermák Ji., Hartman M., Pohořelý M.: Emissions of NO and N₂O in Pressurized Bed Combustion of Subbituminous Coals. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 5, p. 232, Prague, Czech Republic, 25-29 August 2002.

Laser Chemistry Group

Research staff: J. Polá, V. Dřínek, R. Fajgar, A. Galík, A. Galíková, J. Kupčík, D. Pokorná,
M. Urbanová, K. Vacek
NATO fellow: R. Tomovská

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
- IT laser ablative deposition of silicon monoxide and polymeric films

Research projects

Laser ablation and chemistry of silicon monoxide

(J. Pola, supported by GA CR, grant No. 203/00/1288)

IR laser ablation of silicon monoxide in the presence of gaseous organic compounds (methanol, hydrocarbons) has been studied to explore reactivity of ablated particles towards these compounds. The procedure allows chemical vapour deposition of Si/C/H/O and Si/C/H polymeric films. [Refs. 1, 12]

Laser photolysis and thermolysis of organic and organometallic compounds for fabrication of nano-structures of metals in polymer matrices

(J. Pola, supported by GAAV CR, grant No. A 4072107)

IR laser gas-phase co-pyrolysis of iron pentacarbonyl and silacyclic compounds results in unusual polymerisation of the silacycles affording Fe clusters enveloped by organosilicon polymer. The mechanism of this reaction involves Fe(CO) species-assisted ring cleavage and polymerisation of the silacycle. IR laser thermolysis of dimethyl selenium and selenophene was studied to explore mechanism of these reactions and explain formation of solid Se (Se/C) materials deposited from the gas phase. [Refs. 13, 16]

Laser induced deposition of naked and polymer-embedded metal clusters

(J. Pola, supported by Ministry of Education, Program COST, grant No. OC 523.60)

UV laser gas-phase co-photolysis of tetravinylgermane and carbon disulfide affords chemical vapour deposition of organogermanium films that are produced by co-polymerization of both reactants. UV laser photolysis of gaseous trimethoxysilane yields ultrafine powders of SiO_x materials with low content of carbon and shows an effective removal of carbon moieties from the reactant. [Refs. 6, 9, 17]

Laser deposition of novel polymers and composites

(J. Pola, supported by Ministry of Education, Program KONTAKT No. ME 484)

UV laser co-photolysis of tetravinylgermane (TVG) and carbon disulfide yields aerosol polymer particles and represents a unique incorporation of TVG into polymerizing CS species. IR laser irradiation of CS₂/1,3-disilacyclobutane affords chemical vapour deposition of Si/C/H/S polymer whose formation takes place via co-polymerization of silene and CS₂. [Refs. 15, 22, 24]

Laser control of photochemical reactions for deposition of polymeric nano structures

(J. Pola, supported by Ministry of Education, Program KONTAKT, grant No. ME 483)

UV laser photolysis of 1-buten-3-yne was revealed as molecular extrusion of ethyne as proved by examination of photolysis of deuterium-labeled 1-buten-3-yne. UV laser photolysis of butadiyne affords, depending on irradiation conditions, efficient chemical vapour deposition of unsaturated C/H polymer or hydrogenated carbon. [Ref. 4]

International co-operations

CEA-DSM-DRECAM, Service des Photons, Atomes et Molecules, Saclay, France

Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Łódź, Poland

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

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

Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Russia: IR photolysis of silacycles in the condensed state

National Institute of Materials and Chemical Research, Tsukuba, Japan: Laser control of organic reactions

University of Crete, Heraklion, Greece: Infrared multiphoton photolysis of disiloxanes

Visits abroad

J. Pola: Institute of Materials and Chemical Research, Tsukuba, Japan (2 months)

Visitors

H. Morita, Chiba University, Chiba, Japan

L. Tumanova, Institute of Spectroscopy, Troitsk, Russia

E. A. Volnina, Institute of Petrochemical Research, Moscow, Russia

N. Herlin, CEA-DSM-DRECAM, Service des Photons, Atomes et Molécules, Saclay, France

H. Buerger, Wuppertal University, Wuppertal, Germany

T. Majima, Osaka University, Osaka, Japan

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

M. Santos, Institute of Structure of Materials, CSIC, Madrid, Spain

R. Alexandrescu, Institute of Physics and Laser Devices, Bucharest, Romania

Publications

Original papers

1. Dřínek V., Bastl Z., Šubrt J., Yabe A., Pola J.: IR Laser-Induced Reactive Ablation of Silicon Monoxide in Hydrogen and Water Atmosphere. *J. Mater. Chem.* 12(6), 1800-1805 (2002).
2. Herlin-Boime N., Ténégal F., Bastl Z., Šubrt J., Jursíková K., Blechta V., Pola J.: IR Laser Thermolytic Conversion of Disiloxanes to Polyoxocarbosilane Phase and Silicon Carbide. *J. Mater. Chem.* 12(5), 1568-1572 (2002).
3. Pola J., Bastl Z., Ouchi A.: ArF Laser Photo-Polymeric Films of Acetylene. *Surf. Coat. Technol.* 157(1), 55-58 (2002).
4. Pola J., Bastl Z., Ouchi A., Šubrt J., Morita H.: Atmospheric Pressure Chemical Vapour Deposition of Polycarbosilane Films via UV Laser Polymerization of Ethynyltrimethylsilane. *Surf. Coat. Technol.* 149(2-3), 129-134 (2002).
5. Pola J., Galíková A., Galík A., Blechta V., Bastl Z., Šubrt J., Ouchi A.: UV Laser Photolysis of Disiloxanes for Chemical Vapour Deposition of Nano-Textured Silicones. *Chem. Mater.* 14(1), 144-153 (2002).

6. Pola J., Kupčik J., Blechta V., Galíková A., Galík A., Šubrt J., Kurjata J., Chojnowski J.: Thermally Stable Polyoxocarbosilane Thin Films by Pulsed IR Laser Ablation of Poly[oxy(tetramethyldisilane-1,2-diyl)]. *Chem. Mater.* 14(3), 1242-1248 (2002).
7. Pola J., Santos M., Diaz L., Jursíková K., Bastl Z., Boháček J., Fajgar R., Urbanová M.: IR Laser-Induced Thermolysis of (Chloromethyl)silane: Complex Reaction Involving H_2Si , H_2C : and HClSi : Transients and Yielding Nanostructured Si/C/H Phases. *J. Mater. Chem.* 12(5), 1519-1524 (2002).
8. Santos M., Diaz L., Pola J.: Transient Detection in Infrared Multiphoton Decomposition of (Chloromethyl)silane and 1,3-Disilacyclobutane: Evidence for Cleavage of SiCH_4 Intermediates. *J. Photochem. Photobiol., A* 152(1-3), 17-24 (2002).
9. Tumanova L.M., Tumanov O.A., Pola J., Kupčik J.: Decomposition of Liquid Hexamethyldisiloxane Induced by CO_2 Laser Pulse Heating of Carbon Particles. *Chem. Phys.* 278(1), 31-39 (2002).
10. Urbanová M., Pola J.: UV Laser Photolysis of Silacyclopent-3-ene: Effect of Admixtures on Nature of Chemically Vapour-Deposited Organosilicon Films. *Appl. Organometal. Chem* 16(10), 580-586 (2002).
11. Urbanová M., Pola J.: Infrared Laser-Powered Homogeneous Decomposition of (Chloromethyl)trimethylsilane: 1,2-Cl Shift and Methene Expulsion Yielding Chlorotrimethylsilane. *J. Anal. Appl. Pyrolysis* 62(2), 197-203 (2002).
12. Dřínek V., Bastl Z., Šubrt J., Pola J.: IR Laser-Induced Ablation of Silicon Monoxide in Gaseous Methanol and Hydrocarbons: Organically-Modified Silicon Oxide. *Solid State Sci.*, submitted.
13. Fajgar R., Bastl Z., Šubrt J., Vacek K., Pola J.: IR Laser-Induced Gas-Phase Polymerization of Silacyclopent-3-ene Catalyzed by an In situ Generated $\text{Fe}(\text{CO})$ Species. *Phys. Chem. Chem. Phys.*, submitted.
14. Pola J., Ouchi A., Vacek K., Galíková A., Blechta V., Boháček J.: Nano-Sized Silicone Powders by Megawatt UV laser Photolysis of Disiloxanes. *J. Mater. Sci.*, submitted.
15. Pola J., Tomovská R., Bakardjieva S., Galíková A., Vacek K., Galík A.: Megawatt Laser Photolysis of Trimethyl(vinyloxy)silane: Formation of Nano-sized Crosslinked Polyoxocarbosilane with Superior Thermal Stability. *J. Non-Cryst. Solids*, submitted.
16. Pola J., Urbanová M., Volnina E., Bakardjieva S., Šubrt J., Bastl Z.: Polymer-Stabilized Nano-Sized Tellurium Films by Laser-Induced Chemical Vapour Co-Deposition Process. *J. Mater. Chem.*, in press.
17. Tomovská R., Bastl Z., Boháček J., Pola J.: Laser Photolysis of Trimethoxysilane: Chemical vapour deposition of Nanostructured Silicone Powders with Si-H and Si-OCH_3 Bonds. *Appl. Organometal. Chem.*, submitted.

Patents

18. Ouchi A., Pola J.: Generation of Chalcogenide Elements. Pat. No. 2002-056925. Applied: 02.03.04.
19. Ouchi A., Pola J.: Generation of Chalcogenide Elements. Pat. No. 2002-056926. Applied: 02.03.04.
20. Ouchi A., Pola J., Bastl Z., Vorlíček V., Šubrt J.: Preparation Method of Metal Selenide Thin Films. Applied: 02.11.15.

Conferences

21. Galíková A., Galík A., Pola J.: The Study of Kinetics of Adsorption of Some Compounds on Porous Silicas Using Cahn Recording Microbalances. 29th International Conference

- of Slovak Society of Chemical Engineering, Proceedings, p. 116, Tatranské Matliare, Slovakia, 27-31 May 2002.
22. Morita H., Semba K., Pola J., Šubrt J., Bastl Z.: Gas-Phase Synthesis of Ultra-Fine Particles from a Gaseous Mixture of Tetraethenylgermane and Carbon Disulfide. Annual Meeting on Photochemistry, Book of Abstracts, Kyoto, Japan, 11-13 September 2002.
 23. Pola J., Kupčik J., Jursíková K., Bastl Z., Šubrt J., Papagiannakopoulos P., Díaz L., Magna S.: Laser Induced Chemical Vapour Deposition of Nano-Textured Polyoxocarbosilane and Hydrido(methyl)silicone Powders. Joint COST Action Workgroup Meeting on Individual and Assembled Nanoparticles and Quantum Dots, Book of Abstracts, p. P40, Leuven, Belgium, 25-27 March 2002.
 24. Pola J., Semba K., Morita H.: Gas-Phase Synthesis of fine Particle from Tetravinylgermanium and Carbon Disulfide. 3rd International Symposium on Photoreaction Control and Photofunctional Materials, Book of Abstracts, p. P-89, Tsukuba, Ibaraki, Japan, 18-20 March 2002.

Department of Analytical Chemistry

Head: J. Schraml
Deputy: J. Horáček
Research staff: M. Bártlová, V. Blechta, J. Karban, E. Macháčková, L. Soukupová,
J. Sýkora
Technical staff: J. Lněničková

Fields of research

- NMR spectroscopy
- Chromatographic separation of enantiomers

Applied research

- Analytical services to the research departments of ICPF

Research projects

Structure and spectra of hydroxamic acids and their derivatives under various conditions

(J. Schraml, supported by GA AS CR, grant No. A4072005)

Spectral studies of derivatives of hydroxamic acids under different experimental conditions and states of matter with the aim of determining the dependence of their structure on the environmental conditions. [Refs. 10, 17, 19, 20, 21]

International co-operations

University of Ghent, Ghent, Belgium: Study of Neurotoxins as Food Contaminants
Catholic University of Leuven, Leuven, Belgium: NMR in medicinal chemistry

Teaching

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

Publications

Original papers

1. Almeida F.M.T., Carvalho M.F.N.N., Galvao A.M., Čermák Jan, Blechta V., Pombeiro A.J.L., Shaw B.L.: Cationic Nickel(II) Complexes with Azine Diphosphines - Structural and Electrochemical Study. *Inorg. Chim. Acta* 338, 201-209 (2002).
2. Bártlová M., Opletal L., Chobot V., Sovová H.: Liquid Chromatographic Analysis of Supercritical Carbon Dioxide Extracts of *Schizandra chinensis*. *J. Chromatogr., B* 770(1-2), 283-289 (2002).
3. Budka J., Lhoták P., Stibor I., Michlová V., Sýkora J., Císařová I.: A Biscalix[4]arene-based Ditopic Hard/Soft Receptor for K⁺/Ag⁺ Complexation. *Tetrahedron Lett.* 43(15), 2857-2861 (2002).
4. Grabic R., Pekárek V., Fišerová E., Ullrich J., Karban J., Crhová Š., Tomšej T.: Study of the Effect of Matrix on Formation of PCDD, PCDF, PCB and PCBZ by De novo Synthetic Reactions under Model Laboratory Conditions. *Organohalogen Compd.* 56, 205-208 (2002).
5. Grabic R., Pekárek V., Ullrich J., Punčochář M., Fišerová E., Karban J., Šebestová M.: Effect of Reaction Time on PCDD and PCDF Formation by De novo Synthetic Reactions under Oxygen Deficient and Rich Atmosphere. *Chemosphere* 49(7), 691-696 (2002).
6. Herlin-Boime N., Ténégal F., Bastl Z., Šubrt J., Jursíková K., Blechta V., Pola J.: IR Laser Thermolytic Conversion of Disiloxanes to Polyoxocarbosilane Phase and Silicon Carbide. *J. Mater. Chem.* 12(5), 1568-1572 (2002).
7. Lhoták P., Svoboda J., Stibor I., Sýkora J.: Nitration of Thiocalix[4]arene Derivatives. *Tetrahedron Lett.* 43(41), 7413-7417 (2002).
8. Pola J., Galíková A., Galík A., Blechta V., Bastl Z., Šubrt J., Ouchi A.: UV Laser Photolysis of Disiloxanes for Chemical Vapour Deposition of Nano-Textured Silicones. *Chem. Mater.* 14(1), 144-153 (2002).
9. Pola J., Kupčík J., Blechta V., Galíková A., Galík A., Šubrt J., Kurjata J., Chojnowski J.: Thermally Stable Polyoxocarbosilane Thin Films by Pulsed IR Laser Ablation of Poly[oxy(tetramethyldisilane-1,2-diyl)]. *Chem. Mater.* 14(3), 1242-1248 (2002).
10. Schraml J., Blechta V., Karban J., Míndl J.: NMR Study of E/Z Isomerism in N-alkoxybenzoimidic Acid Derivatives. *Magn. Reson. Chem.* 40, 672-676 (2002).
11. Šťastný V., Lhoták P., Michlová V., Stibor I., Sýkora J.: Novel Biscalix[4]arene-based Anion Receptors. *Tetrahedron* 58(36), 7207-7211 (2002).
12. Bureš M., Pekárek V., Karban J., Fišerová E.: Dehalogenation Properties of Municipal Fly Ash. II. Comparison of Dehalogenation Pathway of Fly Ash and Model Fly Ash with Thermodynamic Calculations. *Environ. Sci. Pollut. Res.*, in press.
13. Jochová M., Punčochář M., Horáček J., Štamberg K., Vopálka D.: Removal of Heavy Metals from Water by Lignite-Based Sorbents. *Fuel*, submitted.
14. Kroutil J., Karban J., Trnka T., Buděšínský M., Černý M.: Preparation of O-, S- and N-Benzyl Derivatives of 1,6-Anhydro-beta-d-hexopyranoses via Aziridine Ring Opening. *Collect. Czech. Chem. Commun.*, in press.
15. Ossen A., De Bruyn A., Schraml J., Herdewijn P., De Keukeleire D.: A Novel Polyhydroxylated Alkaloidal Amine from *Solanum elaeagnifolium* with Beta-Glucosidase- and Neuraminidase Inhibiting Activity. *FEBS Lett.*, in press.
16. Pekárek V., Karban J., Fišerová E., Bureš M., Pacáková V., Večerníková E.: Dehalogenation Properties of the Municipal Waste Incineration Fly Ash. I. General Principles. *Environ. Sci. Pollut. Res.*, in press.

17. Podlaha J., Císařová I., Kvíčalová M., Schraml J.: Self-Assembly of 4-Nitrobenzhydroxamic Acid in the Crystal. *Supramol. Chem.*, submitted.
18. Pola J., Ouchi A., Vacek K., Galíková A., Blechta V., Boháček J.: Nano-Sized Silicone Powders by Megawatt UV laser Photolysis of Disiloxanes. *J. Mater. Sci.*, submitted.
19. Řeřicha R., Blechta V., Soukupová L., Císařová I., Podlaha J., Schraml J.: Interpretation of a Missing Spectral Band: Crystal Structure - Spectra Correlation Involving Very Short OH...O Hydrogen Bonds. *Anal. Chem.*, in press.
20. Schraml J., Blechta V., Soukupová L., Tkadlecová M., Volka V., Mindl J., Exner O.: On the Assignment of ^1H NMR Chemical Shifts in NH-OH Fragments of (Benz)hydroxamic Acid Derivatives. *Magn. Reson. Chem.*, submitted.
21. Schraml J., Tkadlecová M., Pataridis S., Volka K., Soukupová L., Blechta V., Exner O.: Ring Substituted Benzhydroxamic Acids - ^1H , ^{13}C , ^{15}N NMR Spectra and NH - OH Exchange. *Magn. Reson. Chem.*, submitted.
22. Sovová H., Sajfrtová M., Bártlová M., Opletal L.: Near-critical Extraction of Pigments and Oleoresin from Stinging Nettle Laves. *J. Supercrit. Fluids*, submitted.

Theses

23. Sýkora J.: RTG-strukturální analýza konformačního a komplexačního chování calixarenových derivátů. (Czech) X-Ray Structure Analysis of Conformational and Complexational Behaviour of the Calixarene Derivatives. PhD Thesis, VŠCHT, Praha 2002.

Conferences

24. Auerová K., Čermák Jan, Blechta V., Kvíčala J.: 1-Hexyne Cyclotrimerization Catalyzed by Cyclopentadienyl Rhodium(I) Complexes. 13th International Symposium on Homogeneous Catalysis, Book of Abstracts, p. 310, Tarragona, Spain, 03-07 September 2002.
25. Budka J., Lhoták P., Stibor I., Sýkora J., Císařová I.: Cation- π Interactions of Calix[4]arenes: Design of Infinite Tubes in the Solid State. XIIth International Symposium on Supramolecular Chemistry, Program and Abstracts, p. O-42, Eilat, Israel, 06-11 October 2002.
26. Budka J., Sýkora J., Císařová I., Michlová V., Lhoták P., Stibor I.: Ditopic Hard/Soft Receptors for K^+/Ag^+ Complexation: Design of Infinite Channels in the Solid State. 27th International Symposium on Macrocyclic Chemistry, Program, p. PA12, Park City, USA, 23-27 June 2002.
27. Budka J., Sýkora J., Císařová I., Stibor I., Lhoták P.: Cation- π Interactions of Calix[4]arenes with Silver Cation: Solution Versus Solid State. 27th International Symposium on Macrocyclic Chemistry, Program, Park City, USA, 23-27 June 2002.
28. De Bruyn A., Schraml J., Busson R., Sandra K., Stals I., Geysens S., Claeysens M., Van Beeumen J., Contreras R.: Isolation and Identification of Phosphorylated Asparagine-Linked N-Glycans on CBH I from *T. reesei*. 16th European Experimental Nuclear Magnetic Resonance Conference, Book of Abstracts, p. PA20, Prague, Czech Republic, 09-14 June 2002.
29. De Bruyn A., Van der Eycken J., Schraml J., Busson R., Sandra K., Claeysens M., Van Beeumen J., Geysens S., Contreras R.: Phosphorylated N-Glycans of Glycoprotein CBH I from the Gungus *Trichoderma reesei*. XXth International Conference on Magnetic Resonance in Biological Systems, Program, p. PL 368, Toronto, Canada, 25-30 August 2002.

30. Morávek J., Stibor I., Sýkora J., Lhoták P.: Stereoselective and Regioselective Oxidation of Thiacalix[4]arenes. 27th International Symposium on Macrocyclic Chemistry, Program, p. PB12, Park City, USA, 23-27 June 2002.
31. Morávek J., Svoboda J., Sýkora J., Stibor I., Lhoták P.: Upper Rim Nitration/Amination of Thiacalix[4]arenes. 27th International Symposium on Macrocyclic Chemistry, Program, p. PB18, Park City, USA, 23-27 June 2002.
32. Opletal L., Sovová H., Bártlová M.: Metoda extrakce superkritickými tekutinami (SFE) v produkci léčivých látek a ve farmaceutické analýze. (Czech) Supercritical Fluid Extraction (SFE) in Production of Medical Substances and in Pharmaceutical Analysis. XXXI. konferencia Syntéza a analýza liečiv, Book of Abstracts, p. 5, Bratislava, Slovakia, 11-13 September 2002.
33. Sajfrtová M., Sovová H., Bártlová M., Opletal L.: Supercritical Fluid Extraction and Characterisation of *Urtica Dioica* L. Leaves Pigments. 15th International Congress of Chemical and Process Engineering CHISA 2002, Summaries 2, p. 279, Prague, Czech Republic, 25-29 August 2002.
34. Šťastný V., Lhoták P., Stibor I., Petříčková H., Sýkora J.: Crystallographic Study of New Types of Ureido and Amidic Derivatives of (Thia)calix[4]arenes. XIIth International Symposium on Supramolecular Chemistry, Program and Abstracts, p. 1-2, Eilat, Israel, 06-11 October 2002.
35. Sýkora J., Budka J., Lhoták P., Stibor I., Císařová I.: Complexes of 1,3-Alternate Calix[4]arenes with Silver Cation. XIX Congress and General Assembly of the International Union of Crystallography, p. 44, Geneva, Switzerland, 06-15 August 2002.

Miscellaneous

International Advisory Board of ICPF

Prof. R. Billet, Ruhr-University Bochum, Bochum, Germany
Prof. L. S. Fan, Ohio State University, Columbus, USA
Prof. J. Gmehling, University of Oldenburg, Germany
Prof. A. Laurent, LSGC-CNRS-ENSIC, Nancy, France
Prof. A. W. Nienow, University of Birmingham, Birmingham, Great Britain
Prof. J. Y. Oldshue, Oldshue Technologies Inter. Inc., Fairport, USA
Prof. R. Pohorecki, Warsaw Technical University, Warsaw, Poland
Prof. J. J. Ulbrecht, OFI Technology Services, Rockville, USA
Prof. K. Yoshida, University of Tokyo, Tokyo, Japan

Organization of International Conferences and Scientific Meetings

15th Congress of Chemical and Process Engineering CHISA 2002, Prague, 25-29 August 2002

16th European Experimental NMR Conference, Prague, 9-16 June 2002

6th Liblice Conference on the Statistical Mechanics of Liquids, Špindlerův Mlýn, 9-14 June 2002

1st Czech-Finish Aerosol Symposium, Prague, 23-26 May 2002

Memberships in Editorial Boards

J. Drahoš: "International Journal of Multiphase Flow"
J. Drahoš: "Clean Products and Processes"
J. Hetflejš: "Chemické listy"
K. Jeřábek: "Reactive and Functional Polymers"
I. Nezbeda: "Molecular Physics"
R. Ponec: "Advances in Molecular Similarity (JAI Press)"
J. Procházka: "Chemical and Biochemical Engineering"
I. Wichterle: "ELDATA: International Electronic Journal of Physico-Chemical Data"
I. Wichterle: "Chemical Engineering and Technology"

Hála Lectures

- First (1999) Arnošt REISER (Polytechnic University, Brooklyn, New York, US)
"Remembering Eduard Hála"
- Second (2000) Gerhart EIGENBERGER (Universität Stuttgart, Stuttgart, DE)
"Membrane Fuel Cell Systems: A Challenge for Chemical Engineers"
- Third (2001) David AVNIR (Hebrew University, Jerusalem, IL)
"The Measurement of Symmetry and Chirality: Concept and Applications across Chemistry"
- Fourth (2002) William R. SMITH (Guelph University, Guelph, CA)
"Macroscopic- and Microscopic-Level Thermodynamics: Partners in Chemical Engineering Progress"

Notes: