

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 2003

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GENERAL INFORMATION

The Institute of Chemical Process Fundamentals (ICPF) is one of six institutes constituting the Section of Chemical Sciences of the Academy of Sciences of the Czech Republic. The Institute serves as a center for fundamental research in chemical, biochemical, catalytic and environmental engineering. Besides these activities, the Institute acts as a graduate school for PhD studies in the field of chemical 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 21)
Department of Multiphase Reactors (page 29)
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Department of Reaction Engineering in Gas Phase (page 43)
Department of Analytical Chemistry (page 61)

STAFF
(31 December 2003)

Category	Number of Employees
Research	113
Technical	23
Administrative	16
Services	14

BUDGET 2003
(in million Kč; 28 Kč = 1 US\$, approx.)

Institutional support from National Budget	58
Research funds from Grant Agencies	30
Contracts with industry	4

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

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PhD students: P. Bernášek, J. Čermáková, K. Fialová, J. Kříšťál, J. Ondráček, M. Sajfrtová,
P. Svoboda, P. Veverka

Fields of research

- 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 tall oil from wastewaters of paper industry
- Supercritical fluid extraction of natural products; Enzymatic reactions in supercritical CO₂; Solubilities of liquids and solids in dense CO₂ with entrainer
- Relation between the morphology and application properties of polymer catalysts and adsorbents
- Gas capillary condensation in small pores of inorganic membranes and its influence on membrane separation properties

Applied research

- Research and development of three-dimensional electrodes in metal electrowinning and wastewater treatment
- Extraction of fermentation broth
- Refining of plant extracts
- Extraction and refining of secondary industrial resources
- Supercritical fluid extraction of biologically active substances from plants
- Analysis of function of the catalytic reactor for bisphenol A synthesis and research of the catalytic deactivation
- Preparation of corundum support for ceramic membranes

Research projects

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

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

As a part of our basic research we have found that the dynamics of transition of the hydrodynamic regime towards flooding is different from that of recovery of the state existing prior to the flooding. On the basis of this findings the goal of this project is to study the possibilities of operating the counter current packed bed column in the dynamic state forced by imposed changes of the flow rates of either liquid or gas with periodic excursions into the domain beyond the flooding point. [Refs. 10, 19, 20, 22, 23, 28]

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

(A. Heyberger, supported by 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. 5, 9, 13, 38]

Liquid extraction of tall oil

(A. Heyberger, joint project with Institute of Landscape Ecology AS, 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 soap and for separation of the fraction of fatty and resin acids and sterols 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 with supercritical CO₂ modified by ethanol from leaves and roots of stinging nettle (*Urtica dioica* L.), leaves of *Ginkgo biloba*, and leaves and roots of *Leuzea carthamoides*. The research was concentrated on operating condition optimization, phase equilibria for low-polar and polar substances during the extraction from plants, and derivation of mathematical model for the complete extraction process including the effect of mass transfer. [Refs. 15-18, 24, 34-37]

Enzymic catalysis in supercritical carbon dioxide

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

Enzymic modifications of blackcurrant seed oil in supercritical carbon dioxide are studied in a continuous-flow extractor. The aim is to develop an integrated production and product recovery process for the extraction from seed and lipase catalysis in supercritical CO₂. [Ref. 6]

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

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

Influence of variations in the morphology of polymer adsorbents on adsorption and absorption of organic compounds into the polymer skeleton has been studied on series of polymers with different degree of modification of the morphology by additional crosslinking with methylene bridges generated in Friedel-Craft reaction [Ref. 21]. With the help of mathematical modeling of the behaviour of industrial reactor for production of bisphenol A,

the cause of the reactor performance decline was identified and suitable preventive measures were proposed [Ref. 14]. In cooperation with Italian colleagues, the methods were developed for generation of size-controlled metal nanoclusters within swollen polymer networks useful as catalysts [Refs. 1, 2, 7, 11].

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

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

The study was focused on measurements and a description of the mass transport in polymeric and inorganic membranes. Modification of ceramic supports of zeolite membranes and measurements of the separation of binary mixture methane/n-butane on these membranes were done [Ref. 12]. Condensation of vapor in small pores of inorganic membranes and description of a transport mechanism in pores were investigated [Ref. 8]. The other results of the mass transport experiments of organic substances during vapor permeation and pervaporation were published in renowned journals and presented on international conferences [Refs. 3, 4, 29, 31].

International co-operations

AECI, Johannesburg, Republic of South Africa: Extraction of food antioxidants on the basis of phenols

CSIR of Pretoria and Johannesburg, Johannesburg, Republic of South Africa: Liquid-liquid extraction process

Hiroshima University, Hiroshima, Japan: Pervaporation on ceramic membranes

Institute of Chemical Engineering, Sofia, Bulgarian AS: Extraction of trialkylamines; Separation of heavy metals from aqueous solutions using amine extractants; High-pressure phase equilibria

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

Technical University, Bratislava, Slovakia: Polymer supported catalysts

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

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

University of Jammu, Chemistry Department, India: Transport phenomena in pervaporation and vapour permeation of propan-1-ol in polyethylene membrane

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

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

University of Stellenbosh, Stellenbosh, Republic of South Africa: Modelling of back mixing in vibrating-plate extractor

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

Visits abroad

A. Heyberger: University of Durban, AECL, CSIR, Johannesburg, Republic of South Africa (6 weeks)

Visitors

M. Bocevská, University of Skopje, Macedonia
S. Boyadzhieva, Institute of Chemical Engineering, Sofia, Bulgaria
M. Sharma, University of Jammu, Chemistry Department, India
J. Modiba and V. Cukan, CSIR, Johannesburg, Republic of South Africa
D.J. Robinson, Dremco, Inc., Electrowinning Technology, Phoenix, USA

Teaching

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

Publications

Original papers

1. Artuso F., D'Archivio A.A., Lora S., Jeřábek K., Králik E., Corain B.: Nanomorphology of Polymer Frameworks and Their Role as Templates for Generating Size-Controlled Metal Nanoclusters. *Chem. Eur. J.* 9(21), 5292-5296 (2003).
2. Bombi 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 Tests in the Hydrogenation of 2-Ethyl-Anthraquinone to 2-Ethyl-anthrahydroquinone. *J. Mol. Catal. A: Chem.* 194(1-2), 273-281 (2003).
3. 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.* 44(9), 2679-2687 (2003).
4. 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.* 214(2), 293-309 (2003).
5. Procházka J., Heyberger A., Volaufová E.: Sulfuric Acid Extraction with Trialkylamine - Effect of Xylene and n-Octanol as Modifiers. *Ind. Eng. Chem. Res.* 42(21), 5305-5311 (2003).
6. Sovová H., Zarevúcka M.: Lipase-Catalyzed Hydrolysis of Blackcurrant Oil in Supercritical Carbon Dioxide. *Chem. Eng. Sci.* 58(11), 2339-2350 (2003).
7. 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 Bio-Catalysis. Part I. Poly-hydroxyethylmethacrylate-Hydroxypropylmethacrylate-Trimethylolpropanetrimethacrylate. *React. Func. Polym.* 55(1), 21-26 (2003).

8. Uchytíl P., Petříčkovič R., Thomas S., Siedel-Morgenstern A.: Influence of Capillary Condensation Effects on Mass Transport through Porous Membranes. *Sep. Purif. Technol.* 33(3), 273-281 (2003).
9. Procházka J., Heyberger A., Volaufová E.: Extraction Equilibrium of Dicarboxylic Acids with Tertiary Amine in Single and Binary Diluents. *Sep. Sci. Technol.* 39(5), 1075-1093 (2004).
10. Akramov T.A., Svoboda P., Jiříčný V., Staněk V.: Analysis of the Conditions for the Appearance of the "Overshoot" Phenomenon in Counter-Current Packed Columns. *Ind. Eng. Chem. Res.*, submitted.
11. Corain B., Jeřábek K., Centomo P., Canton P.: Generation of Size-Controlled Pd0 Nanoclusters inside of the Nanoporous Domains of Gel-Type Resins: Diverse and Convergent Support to a Strategy of. *Angew. Chem. Int. Ed. Engl.*, in press.
12. 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.
13. Poposka F.A., Procházka J., Nikolovski K., Tomovska R.: Extraction of Tartaric Acid from Aqueous Solutions with Tri-isooctylamine (HOSTAREX A 324). Simulation on the Process in a Reciprocating-Plate Extraction Column. *Bull. Chem. Technol. Macedonia*, submitted.
14. Prokop Z., Hanková L., Jeřábek K.: Bisphenol A Synthesis - Modeling of Industrial Reactor and Catalyst Deactivation. *React. Funct. Polym.*, submitted.
15. Sajfírtová M., Sovová H., Opletal L., Bártlová M.: Near-Critical Extraction of beta-Sitosterol, Scopoletin and Homovanillyl Alcohol from Stinging Nettle Roots. *J. Supercrit. Fluids*, submitted.
16. Sovová H.: Mathematical Model for Supercritical Fluid Extraction of Natural Products and for Extraction Curves Evaluation. *J. Supercrit. Fluids*, in press.
17. Sovová H., Opletal L., Bártlová M., Sajfírtová M., Křenková M.: Supercritical Fluid Extraction of Lignans from Caulomas and Leaves of *Schizandra chinensis*. *J. Supercrit. Fluids*, submitted.
18. Sovová H., Sajfírtová M., Bártlová M., Opletal L.: Near-Critical Extraction of Pigments and Oleoresin from Stinging Nettle Leaves. *J. Supercrit. Fluids*, submitted.
19. Svoboda P., Staněk V.: Theoretical Explanation of Pressure and Holdup Overshoots in Counter-Current Packed Columns. *Ind. Eng. Chem. Res.*, submitted.
20. Svoboda P., Staněk V., Jiříčný V.: Experimental Observation of Overshoot Phenomena Near the Flooding Point of Counter-Current Packed Bed Column. *Ind. Eng. Chem. Res.*, submitted.
21. Veverka P., Jeřábek K.: Influence of Hypercrosslinking on Adsorption and Absorption on or in Styrenic Polymers. *React. Funct. Polym.*, submitted.
22. Vychodilová H., Jiříčný V., Staněk V.: An Experimental Study of Absorption of Oxygen in Water in Co-Current Packed Bed Column by Transient Technique. *Chem. Biochem. Eng. Q.*, submitted.
23. Vychodilová H., Jiříčný V., Staněk V.: Mathematical Models of Absorption of Poorly Soluble Gas in Co-Current Packed Bed Column under Periodically Changing Conditions. *Chem. Biochem. Eng. Q.*, submitted.

Review papers

24. Bártlová M., Sovová H., Opletal L.: Liquid Chromatographic Analysis of Supercritical Carbon Dioxide Extracts of Ginkgo Biloba Leaves. Chem. Listy 97(8), 628-629 (2003).

Patents

25. Jeřábek K., Warshawsky A., Strikovskiy A.: Selektivní sorbent pro separaci iontů těžkých kovů a způsob jeho přípravy. (Czech) Selective Sorbent for Separation of Ions of Heavy Metals and Method for its Preparation. Pat. No. PV 1997 - 3012. Applied: 97.09.24, Patented: 03.01.23.
26. Robinson D.J., MacDonald S.A., Jiříčný V.: Method for the Electrolytic Deposition of Copper in Hydrochloric Solution. Applied: 03.03.04.
27. Robinson J., MacDonald S.A., Jiříčný V., Oldani F., Todaro F., Carettin L., Martelli G.N., Scotti D.: Spouted Bed Electrode Cell for Metal Electrowinning. Applied: 02.11.07.

Conferences

28. Akramov T.A., Staněk V., Jiříčný V., Svoboda P.: Matematicheskoe modelirovanie yavleniya "overshoot" v protivotochnoi kolone. (Russ) Mathematical Modeling of the Overshoot Phenomenon in Counter-Current Column. XVI Vserossiiskaya konferentsiya po khimicheskim reaktoram Chimreactor-16, Sbornik tezisev, p. 223-226, Kazaň, Russia, 17-20 June 2003.
29. Fialová K., Petříčkovič R., Uchytíl P.: Transport Phenomena in Pervaporation and Vapor Permeation of Propan-1-ol and Toluene in Polyethylene Membrane. Membrane Science and Technology Conference PERMEA 2003, Proceedings, p. 150, Tatranské Matliare, Slovakia, 07-11 September 2003.
30. Jandová J., Dvořák P., Jiříčný V., Mráz R.: Recycling of ZnO Flue Dust to Produce Zinc by Hydrometallurgical Routes. 5th International Symposium Honoring Professor Ian M. Ritchie Hydrometallurgy 2003, Proceedings, p. 1593-1603, Vancouver, BC, Canada, 24-27 August 2003.
31. Machková J., Šípek K., Izák P., Friess K.: Sorpce organických látek v polymerech. (Czech) Sorption of Organic Compounds in Polymers. Termodynamika 2003, Sborník abstraktů, p. 1-4, Brejlov, Czech Republic, 12-13 September 2003.
32. Prokop Z., Hanková L., Jeřábek K.: Bisphenol A Synthesis - Modelling of Industrial Reactor and Catalyst Deactivation. 3rd Asia-Pacific Congress on Catalysis, Book of Abstracts, p. 198-199, Dalian, China, 12-15 October 2003.
33. Prokop Z., Hanková L., Jeřábek K.: Bisphenol A Sythesis - Modeling of Industrial Reactor and Catalyst Deactivation. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 79, Tatranské Matliare, Slovakia, 26-30 May 2003.
34. Sajfírtová M., Sovová H.: Supercritical Fluid Extraction of Medicinal Components from Urtica dioica L. 4th European Congress of Chemical Engineering, Topic 12 & 13 Abstracts, p. P-12.2-009, Granada, Spain, 21-25 September 2003.
35. Sajfírtová M., Sovová H.: Izolace léčivých látek z kopřivy superkritickou extrakcí. (Czech) Supercritical Fluid Extraction of Medicinal Substances from Stinging Nettle. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1 (plný text 9 stran na CD-ROM), p. 71, Srní, Šumava, Czech Republic, 20-23 October 2003.
36. Sovová H., Bártlová M., Sajfírtová M., Opletal L.: Supercritical Extraction from Plants: New Model and Extraction Curve Evaluation. 4th European Congress of Chemical

- Engineering, Topic 12 & 13 Abstracts, p. P-12.2-010, Granada, Spain, 21-25 September 2003.
37. Sovová H., Opletal L., Sajfřtová M., Bártlová M.: Izolace léčivých látek z rostlin superkritickou reakcí. (Czech) Supercritical Fluid Extraction of Medicinal Substances from Plants. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1 (plný text 9 stran na CD-ROM), p. 70, Srní, Šumava, Czech Republic, 20-23 October 2003.
 38. Volaufová E., Heyberger A., Procházka J.: Effect of Methyl Isobutyl Ketone as Diluent on Amine Extraction of Sulfuric Acid. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 101, Tatranské Matliare, Slovakia, 26-30 May 2003.

E. Hála Laboratory of Thermodynamics

Head: I. Wichterle
Deputy: K. Aim
Research staff: M. Bendová, J. Linek, M. Lísal, L. Morávková, I. Nezbeda, J. Pavlíček,
M. Předota, J. Slovák, Z. Wagner
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 P–V–T behaviour of liquids at superambient conditions
- Behaviour of liquids at very high pressures
- Thermodynamic modelling and processing of thermodynamic data
- Development of equations of state based on molecular theory
- Perturbation theory and molecular simulation for simple interaction potentials
- Molecular simulations on model fluids and fluid mixtures
- Application of statistical–mechanical models to real fluids
- Molecular modelling of solubility of liquids
- Molecular modelling of supercritical CO₂ + surfactant systems
- Theory of polar compounds
- Study of systems of associated fluids with statistical mechanics and simple models
- Study of hydrophobic interactions

Applied research

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

Research projects

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

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

Computer simulation method of Monte-Carlo at constant enthalpy and constant pressure was successfully applied to direct simulations of processes based on Joule-Thomson expansion at molecular level. The results obtained for real difluoromethane were in excellent agreement with the standard international equation of state. Validity of the practical equation

of state for the model 2-centre Lennard-Jones fluid has been extended to the parametric region of large molecular elongations and dipole moments. Promising results were obtained for a variant of a newly developed perturbed equation of state for real methanol based on the molecular-level primitive model of association. [Refs. 6, 17, 22, 29-31, 37]

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. The apparatus was tested [7] and three systems composed of benzene and C3-alkylbenzenes were measured [Refs. 8, 10, 33–35, 41]. The measurements of systems of acetophenone and propiophenone each with four aromatic hydrocarbons at 25 °C and 55 °C have been carried out.

Molecular modeling of supercritical carbon dioxide–surfactant–solute systems

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

We have used the configurational-bias Monte Carlo method combined with the parallel tempering technique to systematically investigate, using simple molecular models, solvent driven changes in polymer conformations in a supercritical solvent. The solvent was modelled as a square-well fluid, and the polymer was made up of a flexible chain of tangentially touching hard spheres and/or square-well spheres. The simulation results showed that conformation behavior of amphiphilic chains was rather complex and it was not a simple combination of the conformation behavior of the attractive and repulsive chains. [Refs. 1, 4, 5, 18, 38, 39]

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

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

We have used Monte Carlo simulations in combination with the Widom method and examined prediction of Henry's constant for carbon dioxide in water over a broad range of temperatures. Carbon dioxide was modelled using two three-site potential models. For water, we considered a "family" of widely used simple potential models. We also used the staged free-energy perturbation method to further analyze the infinite-dilution chemical potential for carbon dioxide in water at various representative temperatures. [Refs. 6, 29, 36, 37, 40]

Description of liquid-liquid and vapor-liquid equilibria by molecular simulation

(M. Lísal, supported by Ministry of Education, grant No. 2003-16)

We have modelled alternative HFC refrigerants and their mixtures as two- and one-center Lennard-Jones fluids. Using these simple models, we predicted vapor-liquid equilibria of these refrigerants and their mixtures by Gibbs-Duhem integration, and by the reaction Gibbs ensemble Monte Carlo method. The predictions were very good, and of comparable accuracy to those obtained using the Wilson and the UNIFAC thermodynamic-based approaches, even though such approaches use experimental mixture information. [Refs. 17, 32]

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. [Refs. 5, 12, 18]

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. 11]

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

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

Using realistic (transferable) site-site potentials and latest results of molecular theories of fluids, equations of state for fluids are being developed in a uniform form regardless of details of intermolecular interactions. The equations have the form of a perturbed equation about a suitable short-range reference. The used perturbation expansion is based on results of recent investigations of the effect of long-range interactions on the properties of fluids. For the description of the reference, simple short-range (primitive) models that account both for the shape and size of molecules and short-range effects of electrostatic interactions are being developed for selected classes of fluids and their appropriateness and applicability is examined by computer simulations and theory. [Refs. 13, 16, 26]

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

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

Molecular dynamics simulations were conducted to characterize the microstructure of the (110) rutile-aqueous electrolyte interface. Simulation results of the adsorption sites of positive ions agree very well with X-ray data for Rb^+ and Sr^{2+} . MD and X-ray results for Zn^{2+} adsorption are qualitatively consistent, important differences in adsorption heights lead to hypothesis of a more complex adsorption of $\text{Zn}(\text{OH})^+$. The applications of this study are in colloid chemistry (stability of colloid solutions), biochemistry (cell membranes) and geo-environmental engineering. Results have been presented at conferences [Refs. 47-48] and submitted for publication.

High pressure phase equilibria and supercritical extraction

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

Vapour-liquid equilibria were determined in three CO_2 + aliphatic alcohol systems around critical conditions. Data are evaluated with use of the SRK equation of state; similarly, the prediction of high-pressure solubilities in alternative refrigerants was made. Model of supercritical extraction was elaborated and description of its hydrodynamics has been further extended. Supercritical extraction of lignanes, β -sitosterole and skopoletine from natural raw material was performed experimentally. Results were evaluated with use of the proposed model. [Ref. 15; see also Department of Diffusion and Separation Processes, Refs. 15, 16, 36]

State behaviour and phase equilibria in fluid systems

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

Systematic experimental determination of isothermal vapour–liquid equilibria has been carried out in binary and ternary systems composed of selected compounds containing structural groups: alkyl, hydroxyl, etheric, and ketonic. These data enlarge the base for improvement of group contribution methods. The data were supplemented with measurement of molar excess volumes. The method of maximum likelihood has been elaborated with use of new algorithms eliminating solutions at local extremes for correlation of high-pressure data. Another supplement to the vapour–liquid equilibrium bibliography database (13000 references) was updated. [Refs. 2, 23, 25, 27, 49]

Phase equilibria in reacting systems

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

Experiments: the determinations have been carried out on three model systems with esterification reaction, namely acetic acid + alkyl alcohol \leftrightarrow water + alkyl acetate at isothermal conditions (alkyl = methyl, ethyl, isopropyl). Theory: attention has been paid to direct molecular simulation of a general reaction with use of the Reaction Ensemble Monte Carlo (REMC) method. The aim was to increase conversion; modelling was made for ammonia synthesis reaction. [Ref. 54; four papers in preparation]

Research Centre: Behaviour of multiphase systems under superambient conditions

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

The Centre integrates physical chemistry and chemical engineering research with the aim to develop new super-ambient processes based on gas-liquid-solid contacting. It represents reorientation of R&D potential activities towards the advanced fields of multiphase systems under extreme conditions. The innovation is based on further intensification of all hitherto existing contacts and links of the Centre with academia and industry in Europe. The following research topics were studied in 2003:

- (1) Investigation of reaction and osmotic equilibria – molecular simulation of methanol reforming in supercritical water. Novel methodology will apply simulation to the systems by considering equilibria for hydrogen, i.e. occurrence of hydrogen separation during reactions.
- (2) The structure and thermodynamic properties of the primitive models of water were studied using multi-density equation together with several versions of the closure conditions.
- (3) Essential oil and oleoresin were extracted with supercritical carbon dioxide from different parts of yarrow (*Achillea millefolium*). The effect of extraction conditions on extract antioxidant activity will be evaluated.
- (4) Transient mass-transfer processes at low Peclet numbers were investigated. Equations of 3D unsteady convective diffusion were solved semi-analytically to provide a regression model for the auto-calibration mode of electrodiffusion flow diagnostics.
- (5) The effect of entrance flow pulsations on the character of instantaneous velocity fields in the impinging jet was investigated. The results of hot-wire measurements showed that behaviour of the vortex structures observed in the jet can be controlled by changing the flow excitation parameters.

International co-operations

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

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

Institute of Physical Chemistry, Romanian Academy, Bucuresti, Romania: Measurement and prediction of vapour-liquid equilibrium data

University of Guelph, Canada, and University of Leipzig, Germany: Molecular-based prediction of solubility in bulk and confined systems

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

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

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 (11 months)

Visitors

S. Figuerola-Gerstenmaier, Roviro i Vigili Univ., Tarragona, Spain (3 months)

Yu. Kalyuzhnyi, Institute of Condensed Matter Physics, Natl. Acad. Sci. Ukr., Lviv, Ukraine

Teaching

M. Lísal: J. E. Purkyně University, courses: "Parallel programming", "Applications of Molecular Simulations", "Numerical mathematics I", "Numerical mathematics II"

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: J. E. Purkyně University, course "Introduction to kinetic theory"

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

M. Kotrla, M. Předota: CU, course "Advanced computer simulations in many particle systems"

M. Předota: University of South Bohemia, course "Lectures from physics oriented to particle and nuclear physics"

M. Předota: University of South Bohemia, course "Selected lectures from physics"

Publications

Original papers

1. 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.* 29(6-7), 405-412 (2003).

2. 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.* 68(7), 1175-1192 (2003).
3. 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 Temperatures". *Fluid Phase Equilib.* 208(1-2), 261-263 (2003).
4. Lísal M., Hall C.K., Gubbins K.E., Panagiotopoulos A.Z.: Formation of Spherical Micelles in a Supercritical Solvent: Lattice Monte Carlo Simulation and Multicomponent Solution Model. *Mol. Simul.* 29(2), 139-157 (2003).
5. Lísal M., Nezbeda I.: Conformations of Attractive, Repulsive, and Amphiphilic Polymer Chains in a Simple Supercritical Solvent: Molecular Simulation Study. *J. Chem. Phys.* 119(7), 4026-4034 (2003).
6. Lísal M., Smith W.R., Aim K.: Direct Molecular-Level Monte Carlo Simulation of Joule-Thompson Processes. *Mol. Phys.* 101(18), 2875-2884 (2003).
7. Morávková L., Linek J.: Excess Molar Volumes of (Octane + 1-Chloropentane) at Temperatures between 298.15 K and 328.15 K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.* 35(7), 1119-1127 (2003).
8. 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.* 35(7), 1139-1149 (2003).
9. Morávková L., Linek J.: Excess Molar Volumes of (Octane + 1-Chlorobutane) at Temperatures between 298.15 K and 328.15 K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.* 35(1), 113-121 (2003).
10. Morávková L., Wagner Z., Linek J.: (P, V, T, x) Measurements of the System Benzene + 1,3,5-Trimethylbenzene at Temperatures from 298.15 to 328.15 K and at Pressures up to 40 MPa. *Fluid Phase Equilib.* 209(1), 81-94 (2003).
11. Nezbeda I.: Modeling of Aqueous Electrolytes at the Molecular Level: On the Origin of the Structure Breaking and Structure Enhancement Phenomena. *J. Mol. Liquids* 103(Sp. Iss), 309-317 (2003).
12. Předota M., Ben-Naim A., Nezbeda I.: On Independence of the Solvation of Interaction Sites of a Water Molecule. *J. Chem. Phys.* 118(14), 6446-6454 (2003).
13. Slovák J., Nezbeda I.: On Accuracy of Wertheim's Thermodynamic Perturbation Theory for Primitive Models of Water. *Mol. Phys.* 101(6), 789-798 (2003).
14. Slovák J., Tanaka H., Koga K., Zeng X.C.: Computer Simulation of Bilayer Ice: Structures and Thermodynamics. *Physica A* 319, 163-174 (2003).
15. Teodorescu M., Wichterle I.: Modeling of Nitrogen and Carbon Dioxide Solubility in Alternative Fuels at High Pressures Using the Soave-Redlich-Kwong Equation of State. *Chem. Eng. Technol.* 26(9), 992-995 (2003).
16. Vlček L., Slovák J., Nezbeda I.: Thermodynamic Perturbation Theory of the Second-Order: Implementation for Models with Double-Bonded Sites. *Mol. Phys.* 101(18), 2921-2927 (2003).
17. Lísal M., Aim K., Mecke M., Fischer J.: The Equation of State for Two-Center Lennard-Jones Fluids Revised. *Int. J. Thermophys.*, submitted.
18. Lísal M., Nezbeda I.: Conformations of Homopolymer Chains and Their Phase Behavior in a Simple Supercritical Solvent. *Fluid Phase Equilib.*, submitted.
19. Nezbeda I.: Towards a Unified View of Fluids. *Mol. Phys.*, in press.
20. Nezbeda I., Smith W.R.: On the Calculation of the Critical Temperature from the Second Virial Coefficient. *Fluid Phase Equilib.*, submitted.
21. Nezbeda I., Vlček L.: Thermophysical Properties of Fluids: From Realistic to Simple Models and Their Applications. *Int. J. Thermophys.*, submitted.

22. Pavlíček J., Aim K., Boublík T.: Fluids of the Kihara Molecules. II. Binary Mixtures of n-Alkanes. *J. Phys. Chem.*, submitted.
23. Psutka Š., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Propanol, Diisopropyl Ether and 1-Methoxy-2-Propanol. *Fluid Phase Equilib.*, submitted.
24. Slovák J.: Adsorption of Fluids of Pseudo-Hard Bodies and EPM5 Water on Solid Surface: Density Functional Theory. *Mol. Phys.*, in press.
25. Valtz A., Teodorescu M., Wichterle I., Richon D.: Liquid Densities and Excess Molar Volumes for Water + Diethylene Glycolamine, and Water, Methanol, Ethanol, 1-Propanol + Triethylene Glycol Binary Systems at Atmospheric Pressure and Temperatures in the Range of 283.15–363.15 K. *Fluid Phase Equilib.*, submitted.
26. Vlček L., Nezbeda I.: From Realistic to Primitive Models: A Primitive Model of Methanol. *Mol. Phys.*, in press.

Books and monographs

27. Linek J.: Annual Report 2002. 63 pp., Institute of Chemical Process Fundamentals AS CR, Prague 2003.
28. Nezbeda I., Kolafa J., Kotrla M.: Úvod do počítačových simulací. Metody Monte Carlo a molekulární dynamiky. (Czech) Introduction to Computer Simulations. Methods Monte Carlo and Molecular Dynamics. 205 pp., Nakladatelství Karolinum, Praha 2003.

Conferences

29. Aim K., Lísal M., Smith W.R.: Adiabatic Monte Carlo Simulations of Reacting and Non-Reacting Systems. 4th European Congress of Chemical Engineering, Book of Abstracts, p. P-14.1-031, Granada, Spain, 21-25 September 2003.
30. Aim K., Nezbeda I., Vlček L.: A Molecular-Based Equation of State for Methanol. Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications, Book of Abstracts, p. 5, Cambridge, Great Britain, 09-11 April 2003.
31. Aim K., Vlček L., Nezbeda I.: A New Equation of State for Methanol Based on Molecular Theory for Associating Fluids. 4th European Congress of Chemical Engineering, Book of Abstracts, p. P-14.1-032, Granada, Spain, 21-25 September 2003.
32. Budinský R., Vacek V., Lísal M.: Vapor-Liquid Equilibria of Alternative Refrigerants and Their Binary Mixtures by Molecular Dynamics Simulations. 15th Symposium on Thermophysical Properties, Boulder CO, USA, 22-27 June 2003.
33. Linek J., Morávková L.: Stavové chování kapalných soustav benzen + C3-alkylbenzen při teplotách 298.15 K až 328.15 K. (Czech) (P, V, T) Behaviour of Benzene + C3-Alkylbenzene Liquid Systems at Temperatures 298.15 K to 328.15 K. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1 (plný text 7 stran na CD-ROM), p. 73, Srní, Šumava, Czech Republic, 20-23 October 2003.
34. Linek J., Morávková L.: Dodatkové molární objemy soustav benzen + isopropylbenzen nebo + 1,2,4-trimethylbenzen nebo + 1,3,5-trimethylbenzen při teplotách mezi 298.15 a 328.15 K. (Czech) Excess Molar Volumes of the Benzene + Isopropylbenzene, or + 1,2,4-Trimethylbenzene, or + 1,3,5-Trimethylbenzene Systems at Temperatures between 298.15 K and 328.15 K. Termodynamika 2003, Sborník abstraktů, p. 1-7, Břežlov, Czech Republic, 12-13 September 2003.
35. Linek J., Morávková L.: (P, V, T, x) Measurements of the Benzene + C3-Alkylbenzene Systems at Temperatures between 298.15 K and 328.15 K. 20th European Symposium on

- Applied Thermodynamics ESAT 2003, Preprints, p. 109-112, Lahnstein, Germany, 08-12 October 2003.
36. Lísal M.: Monte Carlo Simulations in Various Ensembles. *Termodynamika 2003*, Sborník abstraktů, p. 1-5, Břejlov, Czech Republic, 12-13 September 2003.
 37. Lísal M., Aim K., Smith W. R.: Direct Monte Carlo Simulation of Joule-Thomson Expansion and Its Application for Alternative Refrigerant Fluid HFC-32. 20th European Symposium on Applied Thermodynamics ESAT 2003, Preprints, p. 69-72, Lahnstein, Germany, 08-12 October 2003.
 38. Lísal M., Nezbeda I.: Conformations of Single Repulsive, Attractive and Amphiphilic Chains in Normal and Associated Supercritical Solvents: Molecular Simulation Study. *Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications*, Book of Abstracts, p. 62, Cambridge, Great Britain, 09-11 April 2003.
 39. Lísal M., Nezbeda I.: Single Repulsive, Attractive and Amphiphilic Chains in Normal and Associated Supercritical Solvents: Molecular Simulation Study. 15th Symposium on Thermophysical Properties, Boulder CO, USA, 22-27 June 2003.
 40. Lísal M., Nezbeda I., Smith W. R.: Direct Monte Carlo Simulation of Joule-Thomson Processes. *Monte Carlo Methods in the Physical Sciences*, Agenda and Abstracts, Los Alamos, NM, USA, 09-11 June 2003.
 41. 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. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 162, Tatranské Matliare, Slovakia, 26-30 May 2003.
 42. Nezbeda I.: Thermophysical Properties of Fluids: From Simple Models to Applications. *Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications*, Book of Abstracts, p. 70, Cambridge, Great Britain, 09-11 April 2003.
 43. Nezbeda I.: From Simple Models to Applications: Molecular-Based Equations of State for Polar and Associating Fluids. 20th European Symposium on Applied Thermodynamics ESAT 2003, Preprints, p. 55-58, Lahnstein, Germany, 08-12 October 2003.
 44. Nezbeda I.: Thermophysical Properties of Fluids: From Simple Models to Applications. 15th Symposium on Thermophysical Properties, Boulder CO, USA, 22-27 June 2003.
 45. Nezbeda I.: Model-Dependent Restructuring of Water around Hydrophobic Solutes. 81st International Bunsen Discussion Meeting "Interfacial Water in Chemistry and Biology", Velen, Germany, 19-23 September 2003.
 46. Předota M., Ben-Naim A., Nezbeda I.: On Independence of the Solvation of Interaction Sites of a Water Molecule. *Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications*, Book of Abstracts, p. 80, Cambridge, Great Britain, 09-11 April 2003.
 47. Předota M., Chialvo A.A., Cummings P.T.: Structural Characterization of Aqueous Electrolytes in Contact with Rutile Surfaces by Molecular Dynamics. *Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications*, Book of Abstracts, p. 80, Cambridge, Great Britain, 09-11 April 2003.
 48. Předota M., Chialvo A.A., Cummings P.T., Zhang Z., Fenter P., Bedzyk M.J., Sturchio N.C.: Structural Characterization of Aqueous Electrolytes in Contact with Rutile Surfaces by Molecular Dynamics and X-ray Scattering Techniques. 77th ACS Colloid and Surface Science Symposium, Book of Abstracts, p. 1, Atlanta, USA, 15-18 June 2003.
 49. Teodorescu M., Valtz A., Richon D., Wichterle I.: Experimental and Consistent Thermodynamic Modelling of Excess Molar Volumes for Strong Associated Binary

- Systems. 20th European Symposium on Applied Thermodynamics ESAT 2003, Preprints, p. 493-496, Lahnstein, Germany, 08-12 October 2003.
50. Vlček L., Nezbeda I.: Three-Site Extended Primitive Models of Water and Methanol. Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications, Book of Abstracts, p. 108, Cambridge, Great Britain, 09-11 April 2003.
 51. Vlček L., Nezbeda I.: Thermodynamic Properties of Primitive Models from Theory and Simulations. Thermodynamics 2003. Thermodynamics and Statistical Mechanics with Industrial Applications, Book of Abstracts, p. 109, Cambridge, Great Britain, 09-11 April 2003.
 52. Vlček L., Nezbeda I.: Jednoduché modely asociujících kapalin - konstrukce a aplikace. (Czech) Simple Models of Associating Fluids: Construction and Applications. Thermodynamika 2003, Sborník abstraktů, p. 1-8, Břevnov, Czech Republic, 12-13 September 2003.
 53. Wichterle I.: Fázové rovnováhy na počátku milénia. (Czech) Phase Equilibria at Turn of the Millenium. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1, p. 35, Srní, Šumava, Czech Republic, 20-23 October 2003.
 54. Wichterle I., Aim K.: Vapour-Liquid and Chemical Equilibria in Water + Alkyl Alcohol + Acetic Acid + Alkyl Acetate Systems. 20th European Symposium on Applied Thermodynamics ESAT 2003, Preprints, p. 41-44, Lahnstein, Germany, 08-12 October 2003.

Department of Catalysis and Reaction Engineering

Head: M. Zdražil
Deputy: P. Schneider
Research staff: D. Gulková, V. Hejtmánek, K. Jirátová, L. Kaluža, J. Kociánová, R. Ponec,
H. Šnajdaufová, O. Šolcová, Z. Vít
Part time: J. Rymeš
Technical staff: H. Součková, G. Yuzhakov
PhD students: P. Čuba, 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
- Precipitation of ammonium aluminum alum by ammonia

Research projects

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, permoporometry). 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, 7, 8, 21, 29, 36, 47, 49, 50, 51]

Study of early ageing of hardened cement paste

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

Physical properties of the hardened cement paste exhibiting a great impact on practice are basically influenced by the nature of its porous structure. Origin of the pores is closely connected with the early stage of hydration process during which the calcium silicate hydrate (CSH) clusters are formed via nucleation and subsequent grows (solidification). This project focuses on the influence of the water to cement ratio both on the induction time of CSH nucleation and on the evolution of porosity in cement gels. The texture properties are correlated together with changes in electrical conductivity and the induction period of calcium silicate hydrates nucleation. [Refs. 16, 45, 46, 48]

Molybdenum sulfide catalysts promoted by platinum metals

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

Oxidic and sulfided Mo/alumina catalysts were modified by small amounts (0.1-0.8 mass%) of Ir and tested in hydrodesulfurization of thiophene and hydrodenitrogenation of pyridine. The catalysts prepared from sulfided Mo possess higher Ir dispersion, better reducibility and activity [Refs. 12, 31]. Similarly, the same procedures were used for RhMo, RuMo, PtMo and PdMo/alumina combinations. The catalysts displayed synergy of about 3-7 in both test reactions. The RhMo system was best for HDS and the PtMo system for HDN [Ref. 52]. The basic high surface MgO and acidic silica-alumina were used as alternative supports. The RhMo/MgO system possessed similar activity and synergy in HDS as its alumina supported counterpart. However, the HDN activity was lower [Ref. 34]. The silica-alumina synthesized from simple precursors (Na silicate, Al nitrate) without organic templates had very narrow pore size distribution at about 4 nm, high surface area of $490 \text{ m}^2\text{g}^{-1}$ and a good thermal stability [Ref. 53].

Synergistic effects in hydrodesulfurization and oxidation reactions

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

Physical-chemical properties and activity in hydrodesulfurization of thiophene of the catalysts prepared by impregnation of alumina by phosphotungstic acid and its Ni, Fe and Co salts were examined. The activity correlated well with the amount of active species reducible at low temperatures of 100-450 °C. [Refs. 9, 21, 22, 40, 42, 44]

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)

The 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 CO_2 and NH_3 . 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. The most active catalysts in the N_2O decomposition were the calcined Ni_4Al_2 and Co_4Mn_2 hydrotalcite-like compounds. [Refs. 15, 24, 27, 29, 32, 37, 39, 41, 43]

Sulfide hydrotreating catalysts with unconventional supports

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

MgO-supported Mo, CoMo and NiMo sulfide catalysts were prepared by impregnation using slurry MoO_3 /methanol and solutions of Ni and Co nitrates in methanol. The catalysts exhibited very high hydrodesulfurization activity and low hydrodenitrogenation activity in competitive reactions of thiophene and pyridine. The promotion effect for HDS of Ni and Co was higher for MgO-supported MoS_2 catalysts than for conventional Al_2O_3 -supported

catalysts. The specific feature in the TEM images of MgO-supported catalysts as compared to conventional Al₂O₃-supported catalysts were fairly broad MoS₂ slab length distribution and the presence of unusually long MoS₂ slabs [Ref. 2]. The literature and our results on MgO-supported Mo, CoMo and NiMo sulfide hydrotreating catalysts were summarized and critically discussed in the review paper. It was concluded that MgO might be promising support because of its basicity that promotes dispersion of acidic MoO₃ and inhibits coking under reaction conditions. However, the texture of high surface area MgO is not stable during aqueous impregnation and special methods of Mo, Co and Ni must be explored [Ref. 25].

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

(M. Zdražil, supported by GA ASCR, grant No. A4072306)

The MoO₃/Al₂O₃ catalysts with eggshell Mo distribution were prepared by new solvent assisted spreading method: Al₂O₃ extrudates reacted with the slurry MoO₃/H₂O. The profiles were visualized either by sulfidation or by electron probe microanalysis. The dispersion of starting MoO₃ influenced the rate of impregnation (spreading); MoO₃ milled in planetary mill reacted faster than MoO₃ milled in agate mortar mill. [Ref. 38]

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. 4-6, 17, 19]

Production of fertilizers from ammonium aluminum alum

(K. Jiráťová, supported by GA ASCR, grant No. ISB 4072305)

The effect of precipitation conditions of ammonium aluminum alum by ammonia in a laboratory reactor (temperature and pH, rates of mixing and precipitation, ionic strength of solution) on the rheological properties of resulting precipitates slurries were examined. [Refs. 23, 30]

International co-operations

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

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

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

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, 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: Synergistic effects in hydrodesulfurization and oxidation reactions

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

National Centre for High Resolution Electron Microscopy, Delft, the Netherlands:
TEM/HREM microstructure of Mo, CoMo and NiMo sulfide hydrotreating catalysts

Visits abroad

L. Kaluža: Research and Development Westaim Ambeton, Kanada (6 months)

Visitors

Y. Yoshimura, AIST, Tsukuba, Japan

M. Toba, AIST, Tsukuba, Japan

A. Gradovac, Rudjev Boskovic Institute, Zagreb, Croatia

L. Hilaire, University of Strasbourg, Strasbourg, France

A. Spojakina, Institute of Catalysis, Sofia, Bulgaria

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. Besalú E., Ponec R., de Julián-Ortiz J.V.: Virtual Generation of Agents against Mycobacterium tuberculosis. A QSAR Study. *Mol. Divers.* 6, 107-120 (2003).
2. Cinibulk J., Kooyman P.J., Vít Z., Zdražil M.: Magnesia-Supported Mo, CoMo and NiMo Sulfide Catalysts Prepared by Nonaqueous Impregnation: Parallel HDS/HDN of Thiophene and Pyridine and TEM Microstructure. *Catal. Lett.* 89(1-2), 147-152 (2003).
3. Hejtmánek V., Šolcová O., Schneider P.: Gas Permeation in Porous Solids. Two Measurement Modes. *Chem. Eng. Commun.* 190(1), 48-64 (2003).
4. Ponec R., Juzakov G.: Evidence for 5-Center 4-Electron Bonding in (C...H...C...H...C) Array. *J. Org. Chem.* 68(21), 8284-8286 (2003).
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6. Ponec R., Juzakov G., Cooper D.L.: Electron Reorganization in Chemical Reactions. Structural Changes from the Analysis of Bond Order Profiles. *J. Phys. Chem.* 107(12), 2100-2105 (2003).
7. Šolcová O., Schneider P.: Multicomponent Counter-Current Gas Diffusion: Determination of Transport Parameters. *Appl. Catal., A* 244(1), 1-9 (2003).
8. Šolcová O., Šnajdaufová H., Schneider P.: Liquid-Expulsion Perm-Porometry (LEPP) for Characterization of Porous Solids. *Micropor. Mesopor. Mat.* 65(2-3), 209-217 (2003).
9. Spojakina A.A., Jirátová K., Kostova N.G., Kociánová J., Stamenova M.: Volfram/alyumooksidnye katalizatory: vliyanie kationa pri $H_3PW_{12}O_{40}$ na svoistva poverkhnosti i aktivnost' v gidrodesulfirovanii. (Russ) Tungsten Hydrotreating Catalysts I. Counteraction Effect on the Properties of Alumina Supported 12-PW₁₂O₄₀. *Kinet. Catal.* (transl. of *Kinet. Katal.*) 44(5), 1-7 (2003).
10. 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.* 77, 767-778 (2003).
11. Gallegos A., Carbó-Dorca R., Ponec R., Waisser K.: Similarity Approach to QSAR. Application to Antimycobacterial Benzoxazines. *Int. J. Pharm.* 269(1), 51-60 (2004).
12. 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*, 255(2), 321-329 (2003).
13. 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.
14. Girónes X., Carbó-Dorca R., Ponec R.: Molecular Basis of LFER Modelling of Electronic Substituent Effect Using Fragment Quantum Self-Similarity Measures. *J. Chem. Inf. Comput. Sci.*, in press.
15. Kovanda F., Grygar T., Dorničák V., Rojka T., Bezdička P., Jirátová K.: Thermal Behaviour of Cu-Mg-Mn and Ni-Mg-Mn Layered Double Hydroxides and Characterization of Formed Oxides. *Appl. Clay Sci.*, submitted.
16. 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.
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Patents

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32. Čuba P., Kovanda F., JirátoVá K.: Calcined Cu(Ni)MgMn Hydrotalcite-like Compounds: Surface Properties, Reducibility and VOC Combustion Activity. XXXV Symposium on Catalysis, Book of Abstracts, p. 50-51, Prague, Czech Republic, 03-04 November 2003.
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47. Šolcová O., Šnajdaufová H., Schneider P.: Texture of Commercial Porous Solids from Liquid-Expulsion Perm-Porometry (LEPP). 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 185, Tatranské Matliare, Slovakia, 26-30 May 2003.
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 50. Soukup K., Šolcová O.: Gas Diffusion in Porous Solids: Wicke-Kallenbach and Graham's Diffusion Cell. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 188, Tatranské Matliare, Slovakia, 26-30 May 2003.
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Department of Multiphase Reactors

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

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. 4, 5, 7, 10, 19-35]

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. Autocalibration approach to electrodiffusion flow diagnostics, adapted for the low Peclet number transport regimes, was applied to obtain diffusivities, mass-transfer coefficients, and near-to-wall velocity profiles of a viscometric flow of the same polymer solutions. [Refs. 12, 40-42, 44-46]

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: (i) 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. (ii) To propose dimensionless

relations describing the course of particle suspension in the mixing equipments with different geometries. [Refs. 38, 39]

Reaction and transport phenomena in complex homogeneous and heterogeneous systems

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

The project is aimed at the preparation of PhD students for research and production activities in modern areas of chemical, pharmaceutical, biological and process industries. It includes both theoretical and experimental work of 20 students/year of ICT and ICPF in research programs directed to studies of hydrodynamics and transport processes in multiphase tower, stirred and membrane mass exchange systems, homogeneous and heterogeneous reactors and microreactors and to the studies of effects of electric field on chemical and biological systems. [Refs. 17, 35]

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. 6, 8, 11, 36, 37, 43]

Chairmanship of the EFCE Working Party on Multiphase Fluid Flow

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

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

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. Four PhD students stayed in our laboratory during the last year. [Ref. 2]

Research Centre: Behaviour of multiphase systems under superambient conditions

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

The Centre integrates physical chemistry and chemical engineering research with the aim to develop new super-ambient processes based on gas-liquid-solid contacting. It represents reorientation of R&D potential activities towards the advanced fields of multiphase systems under extreme conditions. The innovation is based on further intensification of all hitherto existing contacts and links of the Centre with academia and industry in Europe. The following research topics were studied in 2003:

(1) Investigation of reaction and osmotic equilibria – molecular simulation of methanol reforming in supercritical water. Novel methodology will apply simulation to the systems by considering equilibria for hydrogen, i.e. occurrence of hydrogen separation during reactions.

- (2) The structure and thermodynamic properties of the primitive models of water were studied using multi-density equation together with several versions of the closure conditions.
- (3) Essential oil and oleoresin were extracted with supercritical carbon dioxide from different parts of yarrow (*Achillea millefolium*). The effect of extraction conditions on extract antioxidant activity will be evaluated.
- (4) Transient mass-transfer processes at low Peclet numbers were investigated. Equations of 3D unsteady convective diffusion were solved semi-analytically to provide a regression model for the auto-calibration mode of electrodiffusion flow diagnostics.
- (5) The effect of entrance flow pulsations on the character of instantaneous velocity fields in the impinging jet was investigated. The results of hot-wire measurements showed that behaviour of the vortex structures observed in the jet can be controlled by changing the flow excitation parameters.

International co-operations

University of Nottingham, Great Britain: Acoustic aspects of g-l systems
CNRS UPR 15, Paris, France: Electrodiffusion diagnostics of flow
CRTT, Saint Nazaire, France: Backward-facing step flows, Microfluidics
LEGI / IMG, Grenoble, France: Bubble columns
Institute of Fluid Mechanics, Toulouse, France: Hydrodynamic interactions of bubbles
Martin Luther University, Halle, Germany: Hydrodynamics of bubbly flow
Wageningen University, Wageningen, the Netherlands: Rheology
University of Twente, the Netherlands: Vorticity shedding by bubbles
University of Western Ontario, Canada: Resistance force on buoyant particles
Rovira i Virgili University, Tarragona, Spain: Impinging jets
University of Thessaly, Volos, Greece: Liquid film flows
University of Minho, Braga, Portugal: Multiphase bubble bed reactors
University of Porto, Portugal: Hydrodynamics of g-l-s systems
Institute of Thermophysics, RAS, Novosibirsk, Russia: Diagnostics of multiphase flows
Institute of Nuclear Sciences, Belgrade, Serbia and Montenegro: Impinging jets
Institute of Chemical Engineering, BAS, Sofia, Bulgaria: Gas-liquid reactors for complex rheology fluids
A.V.Luikov Heat & Mass Transfer Institute, Minsk, Belorussia: Electrodiffusion diagnostics

Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)
J. Vejražka: Institute of Fluid Mechanics, Toulouse, France (12 months)

Visitors

P.C. Mena, University of Minho, Braga, Portugal (6 months)
V. Mansurov, ITMO Minsk, Belorussia (3 months)

D. Cvetinovic, Institute of Nuclear Sciences, Belgrade, Serbia and Montenegro (3 months)
K. Argyriadi, University of Thessaly, Volos, Greece (3 months)
K. Serifi, University of Thessaly, Volos, Greece (3 months)
V. Bourdette, Rovira i Virgili University, Tarragona, Spain (1 month)
S. Vlaev, Institute of Chemical Engineering, BAS, Sofia, Bulgaria
K. Kryst, University of Western Ontario, Canada
L. Wren, University of Nottingham, Great Britain

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. Růžička: 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

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2. Höller V., Růžička M., Drahoš J., Kiwi-Minsker L., Renken A.: Acoustic and Visual Study of Bubble Formation Processes in Bubble Columns Staged with Fibrous Catalytic Layers. Catal. Today 79-80, 151-157 (2003).
3. Punčochář M., Drahoš J.: Entropy of Fluidized Bed - a Measure of Particles Mixing. Chem. Eng. Sci. 58(12), 2515-2518 (2003).
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6. Tihon J., Tovčigrečko 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. 33(7), 577-587 (2003).
7. Vlaev S.D., Fialová M.: Bubble Column Bioreactors: Comparison with Stirred Fermenters Based on Local Gas Hold-up Distribution. Can. J. Chem. Eng. 81(3-4), 535-542 (2003).
8. Deslouis C., Tribollet B., Tihon J.: Near-Wall Turbulence in Drag Reducing Flows Investigated by the Photolithography-Electrochemical Probes. J. Non-Newtonian Fluid Mech., submitted.
9. Punčochář M., Drahoš J.: Origin of Pressure Fluctuations in Fluidized Bed. Chem. Eng. Sci., submitted.

10. Růžička M.: Vertical Stability of Uniform Bubble Chain. *Int. J. Multiphase Flow*, submitted.
11. Vejražka J., Marty P.: Measurement of Temperature Field Using Thermochromic Liquid Crystals. *Int. J. Thermal Sci.*, submitted.
12. Wein O.: Viscometric Flow under Apparent Wall Slip in Parallel-Plate Geometry. *J. Non-Newtonian Fluid Mech.*, submitted.
13. Wein O., Tihon J.: Linear Stability of Inclined Film Flows. *Fluid Dyn. Res.*, submitted.

Patents

14. 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.
15. Hájek M., Drahoš J.: Způsob vysoušení a desinfekce knih a papírových materiálů. (Czech) Method of Drying and Disinfection of Books and Paper Materials. Pat. No. PV2002-4272. Applied: 02.12.30.
16. Hájek M., Drahoš J., Vozáb J., Volf V.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Volcanic Origin. Pat. No. PCT/CZ/00/00042. Applied: 00.06.12.

Conferences

17. Bunganič R., Růžička M., Drahoš J.: Různé přístupy k modelování procesu tvorby bublin na ponořených otvorech. (Czech) Different Approaches to Modelling of Bubble Formation Process. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1, p. 129, Srní, Šumava, Czech Republic, 20-23 October 2003.
18. Drahoš J.: Komentář k základním principům "zeleného inženýrství". (Czech) A Commentary on Basic Principles of "Green Engineering". Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1, p. 32, Srní, Šumava, Czech Republic, 20-23 October 2003.
19. Fialová M., Růžička M., Drahoš J.: Effect of Gas Distributor on Character of Homogeneous Bubble Bed in Bubble Column Reactors. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 194, Tatranské Matliare, Slovakia, 26-30 May 2003.
20. Fialová M., Růžička M., Drahoš J.: Effect of Gas Distributor, Column Geometry and Surface Active Additives on Flow Regime Transition in Bubble Column Reactors. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1, p. 131, Srní, Šumava, Czech Republic, 20-23 October 2003.
21. Fialová M., Růžička M., Drahoš J.: Effect of Liquid Phase Properties on Character of the Bubble Bed in Heterogeneous Bubbling Regime in Bubble Column Reactors. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 200, Tatranské Matliare, Slovakia, 26-30 May 2003.
22. Fialová M., Růžička M., Drahoš J.: Factors Influencing Character of Bubble Bed in Bubble Column Reactors. 6th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering, Final Program, p. Session 1A, Vancouver, B.C., Canada, 17-20 August 2003.
23. Fialová M., Růžička M., Drahoš J.: Effect of Gas Distributor on the Formation of Homogeneous Bubbling Regime in Bubble Column. 4th European Congress of Chemical Engineering, Topic 5 Abstracts, p. 1-2, Granada, Spain, 21-25 September 2003.

24. Fialová M., Růžička M., Drahoš J.: Effect of Liquid Phase Properties on the Extent of Homogeneous Bubbling Regime and Gas Holdup in Bubble Column Reactors. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 177, Tatranské Matliare, Slovakia, 26-30 May 2003.
25. Fialová M., Vlaev S.D.: Local Gas Holdup in Viscous Batches in Bubble Column Reactor. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 150, Tatranské Matliare, Slovakia, 26-30 May 2003.
26. Mena P.C., Růžička M., Drahoš J., Večeř M., Wichterle K., Teixeira J.A.: Dvojznačný vliv viskozity na stabilitu homogenní vrstvy bublin. (Czech) Dual Effect of Liquid Viscosity on Uniform Bubble Bed Stability. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1, p. 126, Srní, Šumava, Czech Republic, 20-23 October 2003.
27. Raška P., Kulhánková L., Wichterle K., Růžička M.: Dynamika stoupajících bublin. (Czech) Dynamics of Rising Bubbles. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1 (plný text 7 stran na CD-ROM), p. 127, Srní, Šumava, Czech Republic, 20-23 October 2003.
28. Růžička M., Drahoš J., Fialová M., Wichterle K., Thomas N.H.: Shielding Instability of Bubble Chain. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 183, Tatranské Matliare, Slovakia, 26-30 May 2003.
29. Růžička M., Drahoš J., Fialová M., Wichterle K., Thomas N.H.: Ambiguous Effect of Liquid Viscosity on Bubble Bed Uniformity. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 182, Tatranské Matliare, Slovakia, 26-30 May 2003.
30. Růžička M., Drahoš J., Thomas N.H.: Vertical Stability of Bubble Chain. 5th Euromech Fluid Mechanics Conference, Book of Abstracts, p. 72, Toulouse, France, 24-28 August 2003.
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32. Růžička M., Drahoš J., Thomas N.H.: Rayleigh-Benard Instability of Bubbly Layers. 3rd European-Japanese Two-Phase Flow Group Meeting, Book of Abstracts, p. 1-3, Certosa di Pontignano, Italy, 21-27 September 2003.
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34. Růžička M., Večeř M., Drahoš J., Wichterle K.: Dynamické kritérium stability homogenní vrstvy bublin. (Czech) Dynamic Criterion for Stability of Uniform Bubble Bed. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1, p. 125, Srní, Šumava, Czech Republic, 20-23 October 2003.
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36. Tihon J.: Hydrodynamics of the Solitary Waves Travelling Down a Liquid Film. Workshop on Transport Phenomena with Moving Boundaries, Proceedings, Berlin, Germany, 09-10 October 2003.
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Department of Biotechnology and Environmental Processes

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Fields of research

- Bioremediation of organic pollutants in soil and sewage
- Immobilization of biocatalysts, living cells or enzymes, into organic or organic-inorganic matrices by sol-gel process
- Application of immobilized biocatalysts in optical sensors
- Butadiene-siloxane block copolymers
- Detoxification of noxious halogen-containing substances by biochemical dehalogenation
- Microwave activation of heterogeneous catalytic reactions
- Effect of microwave radiation on photochemical reactions
- Structure, reactivity, and catalytic properties of azine diphosphine complexes of transition metals
- Catalysts for fluorous biphasic media
- New cyclization reaction affording dinitrogen heterocycles
- Generation of new compounds for blood substitutes and other biomedical applications

Applied research

- Microwave drying of books and similar paper-based materials
- Microwave technology of glass melting and glass conditioning
- Complex dehalogenation of PCB contaminated soils, waste water and oils

Research projects

Microbial Degradation of Phenolic Compounds in Water and Sediments

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

In particular, the research was focused on screening of proper strains of microorganisms for field application of biodegradation of chlorophenols. The verification of degrading potential of several selected strains and PCB-degrading bacteria was provided. Efficiency of

biodegradation of chlorophenols was tested in water solution of individual and/or mixture of chlorophenols. [Ref. 38]

Bioencapsulation innovation and technologies

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

Conditions for the entrapment of *Pseudomonas fluorescens* HK44, *Saccharomyces cerevisiae* strain SP4 and plant cells *Nicotiana tabacum* L. BY-2 into tetramethoxysilane prepolymer (TMOS) and composites with alginate have been compared. The growth and cell viability in thick layers were monitored by bioluminescence and 2-D fluorescence spectra. The sensitivity of the cells to the conditions used in layer preparation increased in the sequence: *P. fluorescens* HK44 < *S. cerevisiae* strain SP4 < *N. tabacum* L. BY-2. Cell viability decreased with increasing content of Si in composite matrix. The entrapment into alginate-silica composites resulted in leakage of microbial and yeast cells, however, it had positive effects on the growth and metabolic activity of plant cells. [Refs. 6, 12, 17, 31, 36]

Transformation of liquid polybutadienes to polymeric antidegradants and block copolymers

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

In the starting year of the project, the first triblock poly(butadiene)-poly(dimethylsiloxane) copolymer of the BAB type (B=poly(butadiene)) was prepared with molar masses 1100-800-1100. It was found that, to achieve a narrow molecular weights distribution of the triblock copolymers, which is one of the principal targets of the project, neither butadiene, nor siloxane monomer can be employed, and preformed homopolymers already showing the narrow molar mass distribution must be coupled.

Microwave activation of heterogeneous catalytic reactions

(M. Hájek, supported by ICPF and GA CR grant No. 203/03/H140)

Research has been focused on the microwave activation of heterogeneous catalytic reactions in liquid phase where reactants are transparent to microwaves and the catalyst is only compound which couples with microwaves. It was found that reaction can be accelerated when the surface of catalyst is superheated. [Refs. 13, 28]

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 to glass conditioning. [Refs. 15, 26, 27]

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 and compared to reactions under conventional UV radiation. [Refs. 1, 5]

Microwave drying of books

(M. Hájek, supported by ICPF)

New technology of microwave drying of books and paper-based materials has been optimised and applied for patent protection in EU, USA and Canada. [Ref. 2, 20]

New cyclization reaction affording dinitrogen heterocycles

(V. Církva, supported by GA CR, grant No. 203/02/0306)

The cyclization reaction leading to trifluoromethylated Peganine analogues has been studied using microwave radiation. It was found that regioselectivity in the lactam ring closure and diastereoselectivity in substituent configuration were affected.

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 fluorous synthons, bis(perfluoroalkylethyl)acetylenes were synthesized. Model experiments were made towards the preparation of cyclopentadienes with more than three fluorous ponytails. The key dehydration step in the synthesis of perfluoroalkyltetramethylcyclopentadienes was optimized. [Refs. 9, 24, 33]

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 of styrene with aryl bromides and activated aryl chlorides catalyzed by various palladium complexes including chloro-amido palladium(II) diphosphinoazine complexes was studied under conditions of low catalyst loading in sealed ampoules. Maximum TON of about 680 000 was achieved for 4-bromobenzonitrile. Selectivities of products formation were also examined. New coordination mode of diphosphinoazines, viz. (E,E)-tetracoordination was identified in a novel unusual palladium diphosphinoazine complex with axial chirality. Several complexes of diphosphinoazines with Rh(I) and Rh(III) were prepared and characterized by multinuclear NMR and X-ray diffraction. [Refs. 16, 18, 32]

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)

Bioluminescent bioreporter *Pseudomonas fluorescens* HK44, the whole cell bacterial biosensor that responds to naphthalene and its metabolites via the production of visible light, was immobilized into silica matrix by sol-gel technique. The bioluminescence intensities were measured in maximum of the bioluminescence band at $\lambda = 500$ nm. The immobilized cells

(> 10^5 cells per g silica matrix) produced light after induction by salicylate (conc. > 10^{-4} g/l), naphthalene and aminobenzoic acid. The bioluminescence intensities induced by 2,3-dihydroxynaphthalene, 3-hydroxybenzoic acid and 4-hydroxybenzoic acid were comparable to negative control. The cells in silica layers on glass slides produced light in response to presence of an inductor at least 8 months after immobilization, and >40 induction cycles. The results showed that these test slides could be used as assays for multiple determination of water pollution. [Refs. 7, 8]

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. ICPF has taken part in testing of oxygen sensitivity of ruthenium complex and enzyme immobilized into the novel, highly stable and UV-curable material ORMOCER. This material was synthesized in Fraunhofer-Institut fuer Silicatforschung Wuerzburg (Germany).

International co-operations

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

Center for Environmental Biotechnology University of Tennessee USA: Improved biomaterials for the encapsulation of living cells

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

Visitors

H. Hidaka, Meisei University, Tokyo, Japan

S. Shimazu, Department of Materials Science, Chiba University, Japan

Teaching

F. Kaštánek: ICT, course "Bioengineering"

Publications

Original papers

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14. Marseaut S., Debourg A., Dostálek P., Votruba J., Kuncová G.: Biosorbent of Heavy Metals with Silica Matrix. *Int. Biodeterior. Biodegrad.*, submitted.
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 26. Hájek M.: Microwave Technology of Glass Melting. Annual Meeting of the Scandinavian Society of Glass Technology, Abstracts, p. 2, Marienhamn, Finland, 01-03 June 2003.
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Deputy: V. Ždímal

Research groups

Aerosol Laboratory
Group of Hydrodynamics and Chemistry of Incineration
Laboratory of Systems with Fluidized Bed and High Temperature Gas Cleaning
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

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. 1, 5-7, 14, 15, 35-37]

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. 12, 19-21, 31, 32, 34]

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

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

The objective of the project is to study human exposure from air-pollution compounds that account for two important pathways exposure (inhalation and dermal absorption), and to quantify exposure specifically for particulate matter and chloroform in several European urban areas. The scientific aim is to develop science-based methods for quantification of exposure. The environmental and policy-relevant product is the implementation of these methods in conjunction with a robust multiphase modelling environmental management system. [Refs. 17, 18, 30]

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 , V_2O_5/SiO_2 , Cu/SiO_2 , Fe/TiO_2 . The particle morphology, crystallinity and chemical composition are examined by SEM, TEM, SAED, XRD and EDS. The project also includes a mathematical modelling of some particular phenomena of the process of particle formation by CVD. [Refs. 3, 9, 10, 16, 24, 27, 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. 2-4, 8, 9, 22-27]

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

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

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

Comprehensive size resolved characterization of atmospheric particulate matter in Prague

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

The goal of the project is comprehensive characterization of atmospheric aerosol in Prague. For this purpose concurrent sampling on two sites is performed using cascade impactors, SMPS systems, nano-SMPS and APS together with filter based sampling, yielding particle mass and number size distributions. The relations between size and composition is studied using PIXE, PIGE, INAA, ICP-MS, IC, AAS, and GC-MS analyses. The data together with the available source fingerprints are used in main aerosol sources identification. Further, the relation between aerosol mass and particle number size distributions and composition and atmospheric conditions is also analysed. The project is solved in collaboration with Charles University, Prague and Nuclear Physics Institute AS CR. [Ref. 29]

Nucleation studies using diffusion chambers. Atmospheric Aerosol Measurements - Instruments Intercomparison

(V. Ždímal, supported by Ministry of Education, grant No. ME699, program KONTAKT)

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

Light-induced nucleation from supersaturated vapors

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

The aim of this cooperative linkage project is fundamental and applied research in the field of homogeneous and light-induced nucleation. A new experimental technique will be

used, developed especially for the investigations of light-induced nucleation in the diffusion cloud chamber. Substances showing very intriguing properties, e.g. sulphur, will be studied. The very complex phase behaviour of sulphur will be taken into account including its tendency to form stable oligomers in the vapour phase, and the presence of so called lambda point at which many physical properties of sulphur change dramatically.

International co-operations

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

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

The Johns Hopkins University, Baltimore, USA: Light-induced nucleation from supersaturated vapors

Institute of Physical Chemistry Russian Academy of Sciences, Moscow, Russia: Non-equilibrium phenomena on the solid-gas boundary

Karpov Institute of Physical Chemistry, Aerosol Department, Moscow, Russia: Nucleation processes studied in diffusion chambers

Visitors

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

J.M. Mäkelä, Institute of Physics, Tampere University of Technology, Tampere, Finland

Publications

Original papers

1. 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.* 37(2), 195-208 (2003).

2. Levdansky V.V., Smolík J.: Influence of the Temperature Distribution on Chemical Deposition in Internal Problems. *J. Eng. Phys. Therm.* 76(1), 168-172, 2003 (Translated from *Inzh.-Fyz. Zh.* 76(1) 142-145 (2003)).
3. Levdansky V.V., Smolík J., Moravec P.: Trapping of Molecules by Aerosol Particles in Physical and Chemical Deposition. *Int. Commun. Heat Mass Transfer* 30(4), 545-552 (2003).
4. Levdansky V.V., Smolík J., Moravec P.: Massoperenos i zakhvat primesnogo komponenta pri osazhdenii iz gazovoi fazy. (Russ) Mass Transfer and Trapping of the Impurity Component in Deposition from Gas Phase. *Inzh.-Fiz. Zh.* 76(5), 87-91 (2003). (Translated into *J. Eng. Phys. Therm.* 76(5), 1055-1060, (2003))
5. Smolík J., Ždímal V., Schwarz J., Lazaridis M., Havránek V., Eleftheriadis K., Mihelopoulos N., Bryant C., Colbeck I.: Size Resolved Mass Concentration and Elemental Composition of Atmospheric Aerosols over the Eastern Mediterranean Area. *Atmos. Chem. Phys. Discuss.* 3, 2547-2573 (2003).
6. Smolík J., Ždímal V., Schwarz J., Lazaridis M., Havránek V., Eleftheriadis K., Mihelopoulos N., Bryant C., Colbeck I.: Size Resolved Mass Concentration and Elemental Composition of Atmospheric Aerosols over the Eastern Mediterranean Area. *Atmos. Chem. Phys.* 3, 2207-2216 (2003).
7. Lazaridis M., Spiridaki A., Solberg S., Kallos G., Svendby T., Flatoy F., Drossinos I., Housiadas C., Smolík J., Colbeck I., Varinou M., Ždímal V.: Modelling of Combined Aerosol and Photooxidant Processes in the Mediterranean Area. *Water, Air, Soil Pollut.*, submitted.
8. Levdansky V.V., Smolík J., Moravec P.: Polymolekulyarnye plenki na poverkhnosti aerazol'nykh chastits. (Russ) Polymolecular Films on the Surface of Aerosol Particles. *Inzh.-Fiz. Zh.*, submitted.
9. Levdansky V.V., Smolík J., Moravec P.: Critical Size of Aerosol Particles in the Resonance Radiation Field. *Int. Commun. Heat Mass Transfer*, submitted.
10. Moravec P., Smolík J., Levdansky V.V.: Preparation of Al₂O₃-SiO₂ Fine Particles by CVD Method in Tube Flow Reactor. *Powder Technol.*, submitted.
11. Schwarz J., Smolík J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate Emissions from Fluidized Bed Combustion with Fly Ash Recirculation of Czech Lignite with and without Calcareous Additives. *Fuel Process. Technol.*, submitted.
12. Smolík J., Lazaridis M., Moravec P., Schwarz J., Zaripov S.K., Ždímal V.: Indoor Aerosol Particle Deposition in an Empty Office. *Aerosol Sci. Technol.*, submitted.
13. 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 IRSM AS CR, Series AB No. 11*, 37-43 (2003).
14. 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

15. 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*, Kluwer Academic Press, in press.
16. Moravec P., Smolík J., Levdansky V.V., Keskinen H.: CVD Synthesis of Multicomponent Nanosized Particles in an Externally Heated Tube Flow Reactor. In: *Nanostructured*

Materials and Their Applications. (Szymanski W.W., Wagner P.E., Itoh M. Eds.), Facultas Verlags, Wien 2004, pp. 9-19.

Conferences

17. Bryant C., Colbeck I, Smolík J., Eleftheriadis K., Housiadas C., Braniš M., Helmig C., Drossinos Y., Hollander W., Petrakis M., Lazaridis M.: Urban Indoor-Outdoor Aerosol Measurements at Selected Residential Sites within Europe. 14th Annual Conference Held at Reading University Programme, Abstracts [Journal of Aerosol Science, 34(11), 1603, 2003], Reading, UK, Great Britain, 02-03 April 2003.
18. Coulson G., Bartonova A., Bohler T., Broday D.M., Colbeck I, Floisand I., Fudala J., Hollander W., Housiadas C., Lazaridis M., Smolík J.: Health Risks from Pollutants in Domestic Environments: The Urban Exposure Project. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S377-S378, 2003], Madrid, Spain, 31 August - 05 September 2003.
19. Hovorka J., Veron A.J., Schwarz J., Džumbová L., Kugler J., Smolík J.: Tracing of Urban Aerosol Formation by Stable Isotopes of Lead. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S699-S700, 2003], Madrid, Spain, 31 August - 05 September 2003.
20. Lazaridis M., Dahlin E., Hansen J.E., Smolík J., Schmidbauer N., Moravec P., Ždímal V., Hermansen O., Glytsos T., Svendby T., Dye C.: Indoor/Outdoor Particulate Matter Measurements in Two Residential Houses in Oslo, Norway. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S1367-S1368, 2003], Madrid, Spain, 31 August - 05 September 2003.
21. Lazaridis M., Dahlin E., Hanssen J.E., Smolík J., Schmidbauer N., Moravec P., Ždímal V., Hermansen O., Glytsos T., Dye C.: Characterization of Indoor/Outdoor Particulate Matter Characteristics in Two Residential Houses in Oslo, Norway. GNEST Conference, Book of Abstracts, p. 248, Lemnos, Greece, 08-10 September 2003.
22. Levdansky V.V., Smolík J.: Kinetics of Uniform Thin Film Deposition in Internal Problems. European Vacuum Congress EVC-8, Abstracts, p. 193, Berlin, Germany, 23-26 June 2003.
23. Levdansky V.V., Smolík J., Moravec P.: Condensation Growth of Nanoparticles and Impurity Molecule Trapping. International Conference on Nanomaterials and Nanotechnologies (NN 2003), Abstracts, p. 92, Crete, Greece, 30 August - 06 September 2003.
24. Levdansky V.V., Smolík J., Moravec P.: Impurity Molecule Trapping in Growth of Nanoparticles by Deposition from Gas Phase. Physics, Chemistry and Application of Nanostructures 2003, Book of Abstracts, p. 353-356, Minsk, Belarus, 20-23 May 2003.
25. Levdansky V.V., Smolík J., Moravec P.: Effect of Resonance Radiation on Critical Radius of Small Aerosol Particle. E-MRS Spring Meeting 2003, Book of Abstracts, p. H/PIII.15, Strasbourg, France, 10-13 June 2003.
26. Levdansky V.V., Smolík J., Moravec P.: Growth Rate of Small Aerosol Particles in Physical and Chemical Deposition. II International Conference "Colloid-2003", Short Notes, p. 28, Minsk, Belarussia, 20-24 October 2003.
27. Levdansky V.V., Smolík J., Moravec P.: Size Effect in Impurity Molecule Trapping by Growing Aerosol Particles. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S355-S356, 2003], Madrid, Spain, 31 August - 05 September 2003.
28. Moravec P., Smolík J., Levdansky V.V., Keskinen H., Mäkelä J.M.: Synthesis of Zirconia Fine Particles by Vapour-Phase Decomposition of Zirconium tert-Butoxide. European

- Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S283-S284, 2003], Madrid, Spain, 31 August - 05 September 2003.
29. Schwarz J., Smolík J., Hillamo R., Aurela M., Mäkelä T., Brožová I., Šantroch J., Havránek V.: Size Distribution of Spring Suburban Aerosol in Prague. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S711-S712, 2003], Madrid, Spain, 31 August - 05 September 2003.
 30. Smolík J., Barták M., Bartoňová A., Bholer T, Broday D.M., Colbeck I., Coulson G., Floisand I., Fudala J., Hollander W., Housiadis Ch., Lazaridis M.: Evropský Výzkumný projekt URBAN EXPOSURE. (Czech) European Research Project URBAN-EXPOSURE. Ovězení 2003, Program a Sborník konference, p. 236-238, Brno, Czech Republic, 05-07 May 2003.
 31. Smolík J., Moravec P., Schwarz J., Ždímal V., Dahlin E., Drossinos Y., Lapti M., Lazaridis M.: Chování aerosolů ve vnitřním prostředí. (Czech) Indoor Aerosol Behaviour. Ovězení 2003, Program a Sborník konference, p. 25-28, Brno, Czech Republic, 05-07 May 2003.
 32. Smolík J., Moravec P., Ždímal V., Dahlin E., Lazaridis M.: Indoor Particle Concentrations in Family House: Effect of Different Indoor Activities. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S407-S408, 2003], Madrid, Spain, 31 August - 05 September 2003.
 33. Smolík J., Schwarz J., Džumbová L., Havránek V., Kučera J., Sýkorová I.: Trace Elements Behavior During ACFB Combustion of Synthetic Solid Fuel. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S1297-S1298, 2003], Madrid, Spain, 31 August - 05 September 2003.
 34. Smolík J., Schwarz J., Ždímal V., Drossinos Y., Lapi M., Lazaridis M.: Time and Size Resolved Indoor/Outdoor Aerosol Particle Concentrations in an Office. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S409-S410, 2003], Madrid, Spain, 31 August - 05 September 2003.
 35. Smolík J., Ždímal V., Schwarz J., Havránek V., Eleftheriadis K., Lazaridis M., Mihelopoulos N.: Složení atmosférického aerosolu na Krétě. (Czech) Atmospheric Aerosol Composition Measured on Crete. Ovězení 2003, Program a Sborník konference, p. 29-32, Brno, Czech Republic, 05-07 May 2003.
 36. Večeřa Z., Mikuška P., Smolík J., Eleftheriadis K., Bryant Ch., Colbeck I., Lazaridis M.: Monitorování ozonu, oxidu dusičitého, kyseliny dusité, kyseliny dusičné a oxidu siřičitého ve východní oblasti Středomořího moře. (Czech) Measurements of Ozone, Nitrogen Dioxide, Nitrous and Nitric Acids, and Sulphur Dioxide in the Eastern Mediterranean. Ovězení 2003, Program a Sborník konference, p. 55-59, Brno, Czech Republic, 05-07 May 2003.
 37. Večeřa Z., Mikuška P., Smolík J., Eleftheriadis K., Bryant C., Lazaridis I.: Shipboard Measurements of Ozone, Nitrogen Dioxide, Nitrous and Nitric Acids, and Sulphur Dioxide in the Eastern Mediterranean. EGS-AGU-EUG Joint Assembly, Book of Abstracts, p. 05499, Nice, France, 06-11 April 2003.
 38. Ždímal V., Brus D., Stratmann F.: Homogeneous Nucleation Rates of n-Propanol Carrier Gas Effect. European Aerosol Conference 2003, Abstracts [Journal of Aerosol Science, S1069-S1070, 2003], Madrid, Spain, 31 August - 05 September 2003.

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 students: M. Syc, M. Vosecký

Fields of research

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

Applied research

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

Research projects

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)

We studied the influence of combustion regimes and additives, which were injected to the flue gas, on PCDD/F formation. Further, the possibilities of inhibition of de novo synthetic reactions by changing of matrix composition were investigated. Attention has also been paid to the destruction of precursors of toxic compounds. [Refs. 2, 5, 9, 17, 18, 20]

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. Different polychlorinated toxic substances were totally detoxified more than from 99.99%. In the year 2003, the equipment was completed with a dosing device. The successful operation in semi-continuous regime confirmed the possibility of transition to continuous equipment. [Refs. 1, 15, 19]

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, 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. The main finding of the project is the fact that the boilers under study met practically all legislative limits as for POP compounds as for toxic metals. The better results were achieved unequivocally for burner heating boilers. [Ref. 4]

International co-operations

Vrije Universiteit Brussels, Belgium: Formation of POPs

Ishikawajima Harima Heavy Ind Co Ltd, Japan: Dioxin chemistry

Visitors

Dr. R. Weber, Ishikawajima Harima Heavy Ind Co Ltd, Japan

Publications

Original papers

1. Bureš M., Pekárek V., Karban J., Fišerová E.: Dehalogenation Potential of Municipal Waste Incineration Fly Ash. II. Comparison of Dehalogenation Pathways of Fly Ash and Model Fly Ash with Thermodynamic Calculations. *Environ. Sci. Pollut. Res.* 10(2), 121-125 (2003).
2. Pekárek V., Karban J., Fišerová E., Bureš M., Pacáková V., Večerníková E.: Dehalogenation Potential of Municipal Waste Incineration Fly Ash. I. General Principles. *Environ. Sci. Pollut. Res.* 10(1), 39-43 (2003).
3. Punčochář M., Drahoš J.: Entropy of Fluidized Bed – a Measure of Particles Mixing. *Chem. Eng. Sci.* 58(12), 2515-2518 (2003).
4. Tydlitát V., Ocelka T., Horák J.: Malé kotle pro spalování kapalných paliv v ČR. (Czech) Little Boilers in CR for Burning of Liquid Fuels. *Ochrana ovzduší* 15(35), 20-23 (2003).
5. Bureš M., Pekárek V., Wolf G., Punčochář M.: Thermochemical Quantities of Polychlorinated Biphenyls in Ideal Gas State. *Environ. Sci. Technol.*, submitted.
6. Hartman M., Trnka O., Svoboda K., Veselý V.: Impediment to Gas-Porous Particle Fluidization Due to Liquid Depositing upon the Solids. *Chem. Eng. Commun.*, submitted.
7. Hartman M., Trnka O., Svoboda K., Veselý V.: Thermal Dissociation and H₂S Reactivity of Czech Limestones. *Chem. Pap.*, in press.
8. Jočková M., Punčochář M., Horáček J., Štamberg K., Vopálka D.: Removal of Heavy Metals from Water by Lignite-Based Sorbents. *Fuel*, accepted.
9. 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 $N_2 + 10\% O_2$ Atmosphere under Model Laboratory Conditions. Chemosphere, submitted.
10. Punčochář M., Drahoš J.: Origin of Pressure Fluctuations in Fluidized Bed. Chem. Eng. Sci., submitted.
 11. Schwarz J., Smolík J., Džumbová L., Veselý V., Sýkorová I., Kučera J., Havránek V.: Particulate Emissions from Fluidized Bed Combustion with Fly Ash Recirculation of Czech Lignite with and without Calcareous Additives. Fuel Process. Technol., submitted.
 12. Trnka O., Hartman M., Veselý V.: Charakteristika tlakových fluktuací v různých režimech suspenzí plyn - tuhá látka. (Czech) Characteristics of the Pressure Fluctuations in Different Operation Regimes of Gas-Solid Suspensions. Chem. Listy, submitted.

Review papers

13. Hartman M., Svoboda K., Veselý V., Trnka O., Chour J.: Tepelné zpracování čistírenských kalů. (Czech) Sewage Sludge Thermal Processing. Chem. Listy 97(10), 976-982 (2003).
14. 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 Fluidized Bed. Chem. Listy 97(9), 942-948 (2003).

Patents

15. Pekárek V., Hapala P., Fišerová E.: Způsob dehalogenační detoxifikace halogenovaných aromatických a/nebo cyklických sloučenin. (Czech) Process for Dehalogenative Detoxification of Halogen Aromatic and/or Cyclic Compounds. Pat. No. PV 2003-1220. Applied: 03.04.30.
16. 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

17. Pekárek V.: Technology of Catalytic Dehalogenation of POPs Compounds. International Workshop on the Non-combustion Destruction Technologies of POPs, Lectures, p. 1, Prague, Czech Republic, 15-17 January 2003.
18. Pekárek V.: Scientific Activities of the Dioxin Laboratory at ICPF. PREWIN European Network of Lectures, Lectures, p. 1, Prague, Czech Republic, 15-16 May 2003.
19. Pekárek V., Ocelka T., Grabic R.: Technology of Catalytic Dehalogenation of POPs. 1st Workshop "Persistent Toxic Substances Contamination of the European Region", Book of Abstracts, p. 145-148, Brno, Czech Republic, 10-12 November 2003.
20. Vlková L., Pekárek V., Bureš M.: Porovnání experimentálního průběhu dechlorace pentachlorofenolu s termodynamickým výpočtem na popílku ze spaloven komunálních odpadů. (Czech) Comparison of Pentachlorophenol Experimental Dechloration with Thermodynamic Calculations by Municipal Incineration Waste Fly Ash. Kalorimetrický seminář 2003, Sborník příspěvků, p. 185-187, Suchá Rudná v Jeseníkách, Czech Republic, 26-30 May 2003.

Laboratory of Systems with Fluidized Bed and High Temperature Gas Cleaning

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. 4-8, 11, 14]

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. 3, 5, 7, 8, 12]

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. 5, 8, 10, 12]

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; Waste incineration/gasification

Visits abroad

K. Svoboda: Institute for Energy, Joint Research Centre of European Commission, Petten, the Netherlands (9 months)

Visitors

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

Teaching

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

Publications

Original papers

1. Hartman M., Trnka O.: Calcination of Calcium-Based Sorbents at Pressure in a Broad Range of CO₂ Concentrations. *Chem. Eng. Sci.* 58(14), 3299-3300 (2003).
2. Hartman M., Trnka O., Svoboda K., Veselý V.: Thermal Dissociation and H₂S Reactivity of Czech Limestones. *Chem. Pap.* 57(3), 309-316 (2003).
3. Svoboda K., Pohořelý M., Hartman M.: Effects of Operating Conditions and Dusty Fuel on the NO_x, N₂O and CO Emissions in PFB Co-Combustion of Coal and Wood. *Energy Fuels* 17(4), 1091-1099 (2003).
4. Hartman M., Pohořelý M., Trnka O.: Transport Velocities of Different Particulate Materials in Pneumatic Conveying. *Chem. Eng. Sci.*, submitted.
5. Hartman M., Trnka O., Svoboda K., Veselý V.: Impediment to Gas-Porous Particle Fluidization Due to Liquid Depositing upon the Solids. *Chem. Eng. Commun.*, submitted.
6. Pohořelý M., Svoboda K., Hartman M.: Komůrkový surný dávkovač sypkých materiálů. (Czech) Slide Feeder of Different Particulate Materials. *Chem. Listy*, submitted.

7. Pohořelý M., Svoboda K., Hartman M.: Feeding Smaller Quantities of the Particulate Solids. Powder Technol., submitted.
8. Svoboda K., Hartman M., Pohořelý M., Trnka O.: Modelling of Effects of Operating Conditions and Coal Reactivity on Temperature of Burning Particles in Fluidized Bed Combustion. Acta Montana Ser. B, submitted.
9. 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.
10. Trnka O., Hartman M., Veselý V.: Charakteristika tlakových fluktuací v různých režimech suspenzí plyn - tuhá látka. (Czech) Characteristics of the Pressure Fluctuations in Different Operation Regimes of Gas-Solid Suspensions. Chem. Listy, submitted.

Review papers

11. Hartman M., Svoboda K., Veselý V., Trnka O., Chour J.: Tepelné zpracování čistírenských kalů. (Czech) Sewage Sludge Thermal Processing. Chem. Listy 97(10), 976-982 (2003).
12. 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 97(9), 942-948 (2003).
13. Svoboda K., Hartman M., Trnka O., Čermák Ji.: Vysokoteplotní palivové články, vhodná paliva a možnosti jejich využití. (Czech) High-Temperature Fuel Cells, Their Status, Fuels and Applications. Chem. Listy 97(1), 9-23 (2003).
14. Svoboda K., Fernandez Gutierrez M.-J., Baxter D., Hunter Ch.: N₂O Emissions from Waste and Biomass Incineration Plants. Waste Management, submitted.

Conferences

15. Svoboda K., Hartman M., Baxter D., Hunter C.: Integration of Biomass Gasification with High Temperature Fuel Cells. Second International Conference of Central European Energy, Efficiency and Renewable Energy Sources CEEERES'03, Proceedings, p. 145-155, Prague, Czech Republic, 10-11 November 2003.
16. Svoboda K., Pohořelý M., Hartman M.: Emissions in Pressurized Bed Co-Combustion of a Subbituminous Coal with Wood. 30th International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 80, Tatranské Matliare, Slovakia, 26-30 May 2003.

Laser Chemistry Group

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

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

Research projects

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 with silacyclobutane, silacyclopent-3-ene and 1,3-disilacyclobutane results in novel polymerisation of the silacycles, which affords Fe clusters enveloped by organosilicon polymer. The mechanism of this reaction involves Fe(CO) species-assisted dehydrogenation and polymerisation of the silacycle [Ref. 1]. IR laser thermolysis of dimethyl selenium, dimethyl tellurium, selenophene and tellurophene was studied to elucidate mechanisms of these reactions and explain formation of solid materials deposited from the gas phase [Refs. 5, 12, 14, 17]. UV laser gas phase photolysis of some disiloxanes and alkoxy silanes affords chemical vapour deposition of polymers possessing superior thermal stability [Ref. 3, 4, 7].

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 and IR laser gas-phase co-photolysis and co-pyrolysis of tetramethylgermane and tetramethyltin in the presence of carbon disulfide affords polymeric films containing nanoparticles of germanium and tin sulfides. Examination of solid products from IR laser-induced co-pyrolysis of ferrocene (or iron pentacarbonyl) and disiloxanes revealed that these materials are iron nanoparticles embedded in polyoxacarbosilane and that they have superparamagnetic behaviour. [Ref. 13]

Laser deposition of novel polymers and composites

(J. Pola, supported by Ministry of Education, Program KONTAKT, grant No. ME 612)

N₂ laser-induced gas-phase co-photolysis of tetraethenylgermane (TEG) and carbon disulfide yields polymeric aerosol particles and represents a unique incorporation of TEG into polymerizing CS species [Ref. 10]. IR laser irradiation of gaseous CS₂/1,3-disilacyclobutane affords chemical vapour deposition of solid polythiasilacarbosilane films whose formation takes place via co-polymerization of silene and CS₂ [Ref. 16]. UV laser photolysis of CS₂-C₂H₄ mixtures in the gaseous phase represents the first example of copolymerization of carbon disulfide with common monomer and yields novel polymers in which (CS₂)_n moieties are interlinked with ethylene units [Ref. 15].

Laser control of photochemical reactions for deposition of polymeric nano structures

(J. Pola, supported by Ministry of Education, Program KONTAKT, grant No. ME 611)

UV laser photolysis of dimethylselenium affords thin films of elemental selenium that react with metallic substrates at room temperature to produce metal selenide interlayer. Reaction between bulk metal and selenium phases has been up to now regarded to proceed only at very high temperatures and this finding reveals high reactivity of selenium films [Ref. 11]. UV laser photolysis of gaseous butadiyne yields polymeric films with high content of sp^2 hybridized carbon, which are promising candidate materials for EPR oximetry.

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

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

UV laser photolysis and IR laser pyrolysis of tetramethyldisilazane and hexamethyldisilazane in the gas phase affords chemical deposition of polycarbosilazane films that undergo hydrolysis in air. Different reaction conditions have been tested to obtain polymeric films possessing different reactivity towards hydrolysis.

Laser ablative and non-ablative treatment of polymers

(J. Pola, unsupported project)

IR laser ablation of poly(ethylene-alt-maleic anhydride) affords deposition of structurally identical films and is entirely different from the conventional pyrolysis of this polymer, wherein the anhydride group gets completely lost. IR laser ablation of poly(ethylene-alt-maleic anhydride) in the presence of sodium silicate affords deposition of novel polymeric films containing COONa groups. [Ref. 2]

Laser-induced decomposition of four-membered silicon heterocycles

(R. Fajgar, supported by ICPF)

The project has started by syntheses of several model compounds as silacyclobutene and 1,1-dialkyl-silacyclobutenes.

Laser ablation of the silicon based materials at low and cryogenic temperatures

(V. Dřínek, supported by ICPF)

IR laser ablation of SiO and SiO₂ in Kr yielded deposits with increased defect density. Reactions of the deposits with H₂, ammonia, methylamine and dimethylamine have been examined.

Dynamics of the system aliphatic amines - alumina

(A. Galíková, A. Galík, supported by ICPF)

The rate of propylene adsorption on alumina using the Cahn recording microbalances has been examined. The effect of several propylene concentrations on the rate of isothermal adsorption and desorption was investigated at 180 and at 320 °C, followed by temperature programmed desorption. The effect of the changes of temperature of isothermal part of experiment was studied in the range of 80 to 450 °C. Very interesting behaviour, in addition to that observed by us earlier, was observed around 130 °C. The modelling of the results by simulation software will follow.

International co-operations

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

- Chiba University, Chiba, Japan: Laser-induced production of novel Ge-incorporating polymers
- Instituto de Estructura de la Materia, CSIC, Madrid, Spain: Studies on IR laser deposition of polycarbosilanes and silicon carbide
- National Institute of Advanced Industrial Research and Technology, Tsukuba, Japan: Laser control of organic reactions
- University of Crete, Heraklion, Greece: Laser and Cl atom - induced chemical vapour deposition of polycarbosilazanes
- King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia: Reactive ablation for deposition of novel polymeric films

Visits abroad

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

Visitors

- H. Morita, Chiba University, Chiba, Japan
- A. Ouchi, National Institute of Materials and Chemical Research, Tsukuba, Japan
- N. Herlin, CEA-DSM-DRECAM, Service des Photons, Atomes et Molecules, Saclay, France
- L. Díaz, Institute of Structure of Materials, CSIC, Madrid, Spain
- R. Tomovska, University of St. Cyril and Methodius, Skopje, Macedonia
- J. Blazevska Gilev, University of St. Cyril and Methodius, Skopje, Macedonia
- D. Spaseska, University of St. Cyril and Methodius, Skopje, Macedonia
- H. M. Masoudi, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia
- A. Kowalewska, Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Łódź, Poland
- A. Dransfeld, M. Flok, V. Cappello, G. Tekautz, Technische Universität, Graz, Rakousko

Publications

Original papers

1. 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 Fe(CO) Species. *Phys. Chem. Chem. Phys.* 5, 3789-3794 (2003).
2. Pola J., Kupčik J., Durani S.M.A., Khavaja E.E., Masoudi H.M., Bastl Z., Šubrt J.: Laser Ablative Structural Modification of Poly(ethylene-alt-maleic anhydride). *Chem. Mater.* 15(20), 3887-3893 (2003).
3. Pola J., Ouchi A., Vacek K., Galíková A., Blechta V., Boháček J.: Megawatt UV laser Photolysis of Disiloxanes: Thermally Stable Polyoxocarbosilane Powders. *Solid State Sci.* 5(8), 1079-1086 (2003).
4. Pola J., Tomovská R., Bakardjieva S., Galíková A., Vacek K., Galík A.: Megawatt Laser Photolysis of Trimethyl(vinyloxy)silane: Formation of Nano-sized Cross-linked

- Polyoxocarbosilane with Superior Thermal Stability. *J. Non-Cryst. Solids* 328(1-3), 227-236 (2003).
5. Pola J., Urbanová M., Volnina E.A., Bakardjieva S., Šubrt J., Bastl Z.: Polymer-Stabilized Nano-Sized Tellurium Films by Laser-Induced Chemical Vapour Co-Deposition Process. *J. Mater. Chem.* 13(2), 394-398 (2003).
 6. Tomovska R., Bastl Z., Vorlíček V., Vacek K., Šubrt J., Plzák Z., Pola J.: ArF Laser Induced Chemical Vapour Deposition of Polythiène Films from Carbon Disulfide. *J. Phys. Chem.* 107(36), 9793-9801 (2003).
 7. Tomovská R., Bastl Z., Boháček J., Pola J.: Laser Photolysis of Trimethoxysilane: Chemical Vapour Deposition of Nanostructured Silicone Powders with Si-H and Si-OCH₃ Bonds. *Appl. Organometal. Chem.* 17(2), 113-119 (2003).
 8. Dřínek V., Bastl Z., Šubrt J., Pola J.: IR Laser-Induced Ablation of Silicon Monooxide in Gaseous Methanol and Hydrocarbons: Organically-Modified Silicon Oxide. *J. Anal. Appl. Pyrolysis*, in press.
 9. Dřínek V., Vacek K., Pola J., Yuzhakov G., Šolcová O., Naumov S.: Characterization of Deposits Produced by TEA CO₂ Pulsed Laser Ablation of Silicon Mono- and Dioxide. *J. Non-Cryst. Solids*, submitted.
 10. Morita H., Semba K., Bastl Z., Šubrt J., Pola J.: N₂ Laser-Induced Formation of Copolymeric Aerosol Particles in a Gaseous Tetraethenylgermane-Carbon Disulfide Mixture. *J. Phys. Chem.*, submitted.
 11. Ouchi A., Bastl Z., Boháček J., Orita H., Miyazaki K., Miyashita S., Pola J.: Room-Temperature Interaction between Laser-Chemical Vapour-Deposited Selenium and Some Metals. *Appl. Surf. Sci.*, submitted.
 12. Pokorná D., Urbanová M., Bastl Z., Šubrt J., Pola J.: Laser-Induced Gas-Phase Pyrolysis of Dimethyl Selenium: Chemical Deposition of Selenium and Poly(selenoformaldehyde). *J. Anal. Appl. Pyrolysis*, in press.
 13. Pola J., Bastl Z., Vorlíček V., Dumitrache F., Alexandrescu R., Morjan I., Sandu I., Ciupina V.: Laser-Induced Synthesis of Fe-Fe Oxide/Methylmethoxysilicone Nanocomposite. *Appl. Organometal. Chem.*, in press.
 14. Pola J., Pokorná D., Boháček J., Bastl Z., Ouchi A.: Nano-Structured Crystalline Te Films by Laser Gas-Phase Pyrolysis of Dimethyl Tellurium. *J. Anal. Appl. Pyrolysis*, in press.
 15. Tomovska R., Urbanová M., Fajgar R., Bastl Z., Šubrt J., Pola J.: UV Laser-Induced Gas-Phase Co-Polymerization of Carbon Disulfide and Ethene. *Macromol. Rapid Commun.*, in press.
 16. Urbanova M., Pola J.: IR Laser Decomposition of 1,3-Disilacyclobutane in Presence of Carbon Disulfide: Chemical Vapour Deposition of Polythiacarbosilane. *J. Anal. Appl. Pyrolysis*, submitted.
 17. Urbanová M., Pokorná D., Ouchi A., Pola J.: Laser Powered Homogeneous Decomposition of Selenophene and Tellurophene: Evidence on High-Energy Path from trans-Butadienediyl Diradical to Ethyne. *Tetrahedron Lett.*, submitted.

Patents

18. Ouchi A., Pola J.: Generation of Chalcogenide Elements. Pat. No. 2002-056925. Applied: 02.03.04.
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20. Ouchi A., Pola J., Bastl Z., Vorlíček V., Šubrt J.: Preparation Method of Metal Selenide Thin Films. Pat. No. 2003-010230. Applied: 03.01.17.

Conferences

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22. Tomovska R., Fajgar R., Bastl Z., Vorlíček V., Vacek K., Šubrt J., Alexandrescu R., Morjan I., Sandu I., Dumitrache F., Ciupina V., Pola J.: Laser Induced Chemical Vapor Deposition of Nanosized Polythiene and Fe/Organosilicon Nanocomposites. International Symposium on Scientific and Industrial Nanotechnology, Book of Abstracts, p. 10-11, Osaka, Japan, 08-09 December 2003.

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, P. Žáček

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. [Ref. 12]

The Influence of Configuration of Aziridine Derivatives of 1,6-Anhydro- β -D-hexopyranoses on their reactivity

(J. Karban, joint project with Faculty of Science, Charles University, supported by GA ČR, grant No. 203/01/0862)

The study of the regioselectivity of aziridine ring cleavage of several epimino derivatives of 1,6-anhydro- β -D-hexopyranoses with various nucleophiles. [Ref. 5]

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

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

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

NMR spectroscopy in solutions

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

Three relatively independent topics are being studied in solution state: $^{29}\text{Si} - ^{13}\text{C}$ spin-spin coupling constants, DOSY, and LC-NMR.

Response of plants to antropogenic stress by selected heavy metals

(J. Schraml, joint project with Czech Agricultural University, supported by GA CR, grant No. 525/02/0301)

Identification of selected carotenoids and a study of Co^{2+} complexes with methalothioneins by NMR.

Enzymic catalysis in supercritical carbon dioxide

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

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

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. Budka J., Lhoták P., Stibor I., Sýkora J., Císařová I.: Solid State Calix[4]arene Tubular Assemblies Based on Cation- π Interactions. *Supramol. Chem.* 15(5), 353-357 (2003).
2. Bureš M., Pekárek V., Karban J., Fišerová E.: Dehalogenation Potential of Municipal Waste Incineration Fly Ash. II. Comparison of Dehalogenation Pathways of Fly Ash and Model Fly Ash with Thermodynamic Calculations. *Environ. Sci. Pollut. Res.* 10(2), 121-125 (2003).
3. Carré F., Corriu R.J.P., Lancelle-Beltran E., Mehdi A., Reyé C., Guillard R., Sýkora J., van der Lee A.: X-Ray Crystal Structures of Copper(II) and Cobalt(II) Complexes with Schiff Base Ligands. Reactivity towards Dioxygen. *Dalton Trans.* 16, 3211-3215 (2003).
4. Dudič M., Lhoták P., Petříčková H., Stibor I., Lang K., Sýkora J.: Calixarene-Based Metalloporphyrins: Molecular Tweezers for Complexation of DABCO. *Tetrahedron* 59(14), 2409-2415 (2003).

5. Kroutil J., Karban J., Buděšínský M.: Utilization of Nosyepimines of 1,6-Anhydro-beta-D-hexopyranoses for the Preparation of Halogenated Aminosaccharides. *Carbohydr. Res.* 338(24), 2825-2833 (2003).
6. Lhoták P., Himl M., Stibor I., Sýkora J., Dvořáková H., Lang J., Petříčková H.: Conformational Behaviour of Tetramethoxythiacalix[4]arenes: Solution versus Solid-State Study. *Tetrahedron* 59(38), 7581-7585 (2003).
7. Lhoták P., Morávek J., Šmejkal T., Stibor I., Sýkora J.: Stereoselective Oxidation of Thiacalix[4]arenes with the $\text{NaNO}_3/\text{CF}_3\text{COOH}$ System. *Tetrahedron Lett.* 44(39), 7333-7336 (2003).
8. Lhoták P., Zieba R., Hromádka V., Stibor I., Sýkora J.: Neutral Guests Complexation with Calix[4]arenes Preorganised by Intramolecular McMurry Reaction. *Tetrahedron Lett.* 44(24), 4519-4522 (2003).
9. Pekárek V., Karban J., Fišerová E., Bureš M., Pacáková V., Večerníková E.: Dehalogenation Potential of Municipal Waste Incineration Fly Ash. I. General Principles. *Environ. Sci. Pollut. Res.* 10(1), 39-43 (2003).
10. Pola J., Ouchi A., Vacek K., Galíková A., Blechta V., Boháček J.: Megawatt UV Laser Photolysis of Disiloxanes: Thermally Stable Polyoxocarbosilane Powders. *Solid State Sci.* 5(8), 1079-1086 (2003).
11. Rakib S., Sghyar M., Rafiq M., Sýkora J., Císařová I., Durand J., van der Lee A.: A Hexagonal Polymorph of $\text{Fe}(\text{HPO}_3\text{H})_3$. *J. Chem. Crystallogr.* 33(3), 219-222 (2003).
12. Schraml J., Blechta V., Soukupová L., Karban J., Mindl J.: Assignment of Chemical Shifts in Benzohydroxamic Acid and Structure of Its Silylated Derivatives by ^{15}N Enrichment. *Magn. Reson. Chem.* 41(8), 626-628 (2003).
13. Čermák Jan, Šťastná L., Sýkora J., Císařová I., Kvičala J.: Trimethylsilylcyclopentadienes with Polyfluorinated Ponytails and Mono- and Bis(η^5 -cyclopentadienyl)-titanium(IV) Complexes Derived from Them. *Organometallics*, submitted.
14. Osson 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.*, submitted.
15. Podlaha J., Císařová I., Kvičalová M., Schraml J.: Self-Assembly of 4-Nitrobenzhydroxamic Acid in the Crystal. *Supramol. Chem.*, submitted.
16. 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.
17. Sajfrtová M., Sovová H., Opletal L., Bártlová M.: Near-Critical Extraction of beta-Sitosterol, Scopoletin and Homovanillyl Alcohol from Stinging Nettle Roots. *J. Supercrit. Fluids*, submitted.
18. 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.
19. Sovová H., Opletal L., Bártlová M., Sajfrtová M., Křenková M.: Supercritical Fluid Extraction of Lignans from Caulomas and Leaves of *Schizandra chinensis*. *J. Supercrit. Fluids*, submitted.
20. Sovová H., Sajfrtová M., Bártlová M., Opletal L.: Near-critical Extraction of Pigments and Oleoresin from Stinging Nettle Leaves. *J. Supercrit. Fluids*, submitted.

Review papers

21. Bártlová M., Sovová H., Opletal L.: Liquid Chromatographic Analysis of Supercritical Carbon Dioxide Extracts of *Ginkgo Biloba* Leaves. *Chem. Listy* 97(8), 628-629 (2003).

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22. Gavlasová P., Kuncová G., Macková M., Karban J., Demnerová K.: Studium aspektů syntézy barevných meziproductů během degradace polychlorovaných bifenyliů bakterií *Pseudomonas* species P2. (Czech) The Study of Coloured Intermediates of Polychlorinated Biphenyls Degradation by *Pseudomonas* species 2. XII. konference mladých mikrobiologů Tomáškovy dny 2003, Sborník abstraktů, p. 1, Brno, Czech Republic, 04-06 June 2003.
23. Sovová H., Bártlová M., Sajfrtová M., Opletal L.: Supercritical Extraction from Plants: New Model and Extraction Curve Evaluation. 4th European Congress of Chemical Engineering, Topic 12 & 13 Abstracts, p. P-12.2-010, Granada, Spain, 21-25 September 2003.
24. Sovová H., Opletal L., Sajfrtová M., Bártlová M.: Izolace léčivých látek z rostlin superkritickou reakcí. (Czech) Supercritical Fluid Extraction of Medicinal Substances from Plants. Jubilejní 50. Konference chemického a procesního inženýrství CHISA 2003, Sborník 1 (plný text 9 stran na CD-ROM), p. 70, Srní, Šumava, Czech Republic, 20-23 October 2003.
25. Šťastná L., Čermák Jan, Sýkora J., Císařová I.: Titanium(IV) Complexes of Fluorinated Trimethylsilylcyclopentadienes. XXXV Symposium on Catalysis, Book of Abstracts, p. 42, Prague, Czech Republic, 03-04 November 2003.

Miscellaneous

International Advisory Board of ICPF

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Hála Lectures

First (1999)	Arnošt REISER (Polytechnic University, Brooklyn, New York, USA) "Remembering Eduard Hála"
Second (2000)	Gerhart EIGENBERGER (Universität Stuttgart, Stuttgart, Germany) "Membrane Fuel Cell Systems: A Challenge for Chemical Engineers"
Third (2001)	David AVNIR (Hebrew University, Jerusalem, Israel) "The Measurement of Symmetry and Chirality: Concept and Applications across Chemistry"
Fourth (2002)	William R. SMITH (Guelph University, Guelph, Canada) "Macroscopic- and Microscopic-Level Thermodynamics: Partners in Chemical Engineering Progress"
Fifth (2003)"	Jakob de Swaan Arons (Delft University of Technology, the Netherlands) "Economy, Ecology and Thermodynamics"