

Academy of Sciences of the Czech Republic

**Institute of Chemical Process
Fundamentals**

Prague

ANNUAL REPORT 2004

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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 Hanika
Deputy Director (Research)	Jiří Drahoš
Deputy Director (Business Administration)	Eva Melková
Scientific Secretary	Jan Linek
Scientific Board Chairman	Karel Aim

DEPARTMENTS

Department of Diffusion and Separation Processes (page 5)
E. Hála Laboratory of Thermodynamics (page 14)
Department of Catalysis and Reaction Engineering (page 22)
Department of Multiphase Reactors (page 30)
Department of Biotechnology and Environmental Processes (page 38)
Department of Reaction Engineering in Gas Phase (page 45)
Department of Analytical Chemistry (page 62)

STAFF
(31 December 2004)

Category	Number of Employees
Research	122
Technical	22
Administrative	18
Services	15

BUDGET 2004
(in million Kč; 24 Kč = 1 US\$, approx.)

Institutional support from National Budget	64
Research funds from Grant Agencies	29
Contracts with industry	5

Abbreviations used throughout the Report

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

Department of Diffusion and Separation Processes

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

Fields of research

- Hydrodynamic study of dynamic behaviour of two-phase co- and counter-current gas-liquid pulse flow in packed bed column
- 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
- Study of the permeation and pervaporation of volatile organic substance (propan-1-ol, toluene)
- Observation of the competitive adsorption on Vycor glass membrane

Applied research

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

Research projects

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

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

As a part of our basic research we have found that the dynamics of transition of the hydrodynamic regime towards flooding is different from that of recovery of the state existing

prior to the flooding. On the basis of this finding the goal of this project is to study the possibilities of operating the counter-current packed bed column in the dynamic state forced by imposed changes of the flow rates of either liquid or gas with periodic excursions into the domain beyond the flooding point. [Refs. 1, 11, 13, 14, 30, 31, 55, 62]

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

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

Project is focused on the research and development of the know-how and method of intensification and safe control of industrial trickle bed reactors. The effect of hydrodynamics of liquid pulse flow on conversion and selectivity of high-pressure hydrogenation process is studied. [Refs. 29, 74]

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, hydrochloric and nitric acids 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. 6, 21]

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.

Enzymatic catalysis in supercritical carbon dioxide

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

Enzymatic modifications of blackcurrant seed oil in supercritical carbon dioxide are studied in a continuous-flow extractor [Ref. 64]. The aim is to develop an integrated production and product recovery process for the extraction from seed and lipase catalysis in supercritical CO₂. The extraction step is studied, partially in cooperation with Bulgarian and Macedonian colleagues, for different plants [Refs. 4, 10, 15, 18, 22-24, 32, 34, 44, 45, 58-60].

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

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

The project is focused on obtaining α - and γ -linolenic acids from blackcurrant seed *via* a new procedure where enzymatic ethanolysis of blackcurrant oil follows after its supercritical fluid extraction from the seed [Ref. 33]. The aim of the project is to obtain variable and controlled α - to γ -linolenic acid ratios in the produced ethyl esters.

Relations between morphology and activity of 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 cross linking with methylene bridges generated in Friedel-Craft reaction [Ref. 12]. 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. 7]. Study of partial neutralization of the acidic group of the ion exchanger by amines with various molecular sizes and of different base strength shown the importance of the local concentration of active groups and demonstrated the inhomogeneity of the acid strength of the active centers of formally homogeneous chemical composition [Ref. 19].

Study of transport phenomena in polymeric membrane during pervaporation

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

Transport of propan-1-ol through a polyethylene membrane during vapor permeation was investigated. Diffusion coefficients, fluxes and sorption isotherms were evaluated from independent experiments for different vapor concentrations. New apparatus, which enables sorption measurements in steady state of the vapor permeation process, was proposed and constructed. Till now, these data were not experimentally available. The determined sorption data were successfully used for the transport description of propan-1-ol in polyethylene membrane by the Fick's first law [Refs. 17, 40-42]. Also the gas transport and sorption in porous membranes were studied [Refs. 5, 25, 26, 36, 37, 63, 65, 66].

International co-operations

CSIR of Pretoria and Johannesburg, Republic of South Africa: Extraction of essential oils from plant raw materials

University of KwaZulu Natal, Republic of South Africa: Liquid-liquid extraction processes

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

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

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

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

University of 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, CSIR of Johannesburg, Republic of South Africa
(5 weeks)

Visitors

S. A. Aleksovski, University of Skopje, Macedonia
J. Dudas, I. Goodwin, CSIR, Johannesburg, Republic of South Africa
P. Moquin, University of Alberta, Canada
R. P. Stateva, Institute of Chemical Engineering, Sofia, Bulgaria

Teaching

K. Jeřábek: ICT, postgraduate course "Preparation of the heterogeneous catalysts"
H. Sovová: ICT, postgraduate course "Properties and application of supercritical fluids"

Publications

Original papers

1. 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.* 43(18), 5899-5903 (2004).
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11. Svoboda P., Staněk V.: Theoretical Explanation of Pressure and Holdup Overshoots in Countercurrent Packed Columns. *Ind. Eng. Chem. Res.* 43(26), 8317-8322 (2004).
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13. 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.* 18(2), 129-136 (2004).
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15. Sovová H.: Mathematical Model for Supercritical Fluid Extraction of Natural Products and Extraction Curve Evaluation. *J. Supercrit. Fluids* 33(1), 35-52 (2005).
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18. Galushko A.A., Sovová H., Stateva R.P.: Solubility of Menthol in Pressurised Carbon Dioxide – Experimental Data and Thermodynamic Modelling. *J. Supercrit. Fluids*, submitted.
19. Holub L., Jeřábek K.: Influence of Partial Neutralization on Catalytic Activity of Ion Exchange Resin. *J. Mol. Catal.*, submitted.
20. Poposka F.A., Procházka J., Nikolovski K., Tomovska R.: Extraction of Tartaric Acid from Aqueous Solutions with Tri-iso-octylamine (HOSTAREX A 324). Simulation on the Process in a Reciprocating-Plate Extraction Column. *Bull. Chem. Technol. Macedonia*, submitted.
21. Procházka J., Heyberger A., Volaufová E.: Effect of Diluents on Sulfuric Acid Extraction with Trialkylamine. *AIChE J.*, submitted.
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23. Sovová H., Aleksovski S.: Mathematical Model for Hydrodistillation of Essential Oils. *Chem. Eng. Sci.*, submitted.
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44. Galushko A.A., Sovová H.: Solubility of Menthol in Supercritical CO₂ - Experimental Measurements. 10th International Summer School of Chemical Engineering, Proceedings, p. 308, Varna, Bulgaria, 24-31 May 2004.
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46. Hanková L., Holub L., Jeřábek K.: Influence of Partial Neutralization on Catalytic Activity of Ion Exchange Resin. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 220, Tatranské Matliare, Slovakia, 24-28 May 2004.
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58. Sajfritová M., Sovová H.: CO₂ Extraction of Medicinal Components from Plants. 10th International Summer School of Chemical Engineering, Proceedings, p. 315, Varna, Bulgaria, 24-31 May 2004.
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61. Staněk V., Katz S., Landefeld A.: AFS Cupola Furnace Model: Current Status and Predictive Capabilities. 2nd International Cupola Conference, Book of Abstracts, p. 1-6, Trier, Germany, 18-19 March 2004.
62. Svoboda P., Staněk V.: Experimental Observation and Model Description of Overshoot Phenomena in the Countercurrent Packed Bed Column Near the Flooding Point. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 2, p. 440, Praha, Czech Republic, 22-26 August 2004.
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65. Yang J., Čermáková J., Uchytíl P., Hamel C., Seidel-Morgenstern A.: Mass Transport Study of Combined Gas Phase and Surface Diffusion in Porous Glass Membranes. 6th International Conference on Catalysis in Membrane Reactors, Book of Abstracts, p. 136, Lahnstein, Germany, 06-09 July 2004.
66. Yang J., Čermáková J., Uchytíl P., Hamel C., Seidel-Morgenstern A.: Adsorption, Gas Phase Transport and Surface Diffusion in Porous Glass Membranes. 8th International Conference on Inorganic Membranes, Proceedings, p. 446-449, Cincinnati, Ohio, USA, 18-22 July 2004.
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E. Hála Laboratory of Thermodynamics

Head: I. Wichterle
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Research staff: M. Bendová, J. Linek, M. Lísal, L. Morávková, I. Nezbeda, J. Pavlíček,
J. Slovák, Z. Wagner
Part time: M. Předota
Technical staff: S. Bernatová, Š. Psutka
PhD students: A. Babič, J. Jirsák, 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
- Molecular simulations of chemically reacting systems in nanoporous materials

Applied research

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

Research projects

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

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

Validity of the practical equation of state for the model 2-centre Lennard-Jones fluid has been successfully extended to the parametric region of large molecular elongations and dipole moments. Promising results were obtained for variants of a newly developed perturbed equation of state for real methanol based on the molecular-level primitive model of association. First attempts to extend the approach to describe fluid phase equilibrium in

binary methanol + carbon dioxide mixture were made. To this end the database for the system was supplemented by newly measured vapour–liquid equilibrium data. [Refs. 5, 36–38]

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 measurements of the systems of acetophenone with benzene, or toluene, or 1,3-xylene, or 1,3,5-trimethylbenzene and propiophenone with benzene, or toluene, or ethylbenzene, or butylbenzene at 298.15 K and 328.15 K and at atmospheric pressure have been carried out. Then the P–V–T behaviour of the system toluene + propiophenone has been measured along five isotherms between 298.15 K and 328.15 K and at pressures up to 40 MPa and correlated. In addition to it, the systems of decane with four aromatic hydrocarbons along five isotherms and atmospheric pressure have been measured. [Refs. 22–24, 40, 41]

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. We have also studied potential applications of micelles as nanochemical devices. [Refs. 6, 7, 34, 43, 45]

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. We have also developed a novel simulation tool, expanded ensemble osmotic molecular dynamics, to study open (at fixed total chemical potential) electrolyte solutions. [Refs. 8, 9, 44]

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. We have also extended validity of the equation of state for the model two-center Lennard–Jones fluid to the parametric region of large molecular elongations. [Refs. 3, 5]

Molecular model of aqueous solutions of electrolytes and its application

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

The problem of a shortening the Coulombic interactions was investigated with respect to a possibility to develop a theory. Various possibilities were considered and these are summarized, along with a set of recommendations, in [Ref. 35]. The main focus in 2004 was on the determination of the potential of mean force and its differences/similarities in the full and short–range models [Ref. 32]. In addition to these topics, the solvent itself, i.e., water was also examined both from the point of view of best realistic Hamiltonians available [Refs. 8, 9] and primitive models [Ref. 18].

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

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

Methodology to construct primitive models for any given realistic Hamiltonian was completed [Refs. 12, 19, 26]. The construction of the models was then followed by investigations of their thermodynamic properties and their theoretical description by means of the thermodynamic perturbation theory [Ref. 18].

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. Detailed analysis of all types of donor and acceptor hydrogen bonds involving any of the surface O or H atoms was carried out, resolving number of hydrogen bonds and their lengths (related to bond strength) separately for each surface species. The obtained results were compared with MUSIC model assumption on number of hydrogen bonds of model rutile surface. Structural data of Li^+ , Cs^+ , Y^{3+} and F^- ions at the neutral and negatively charged rutile surfaces were collected by molecular dynamics simulations and analysed. The applications of this study are in colloid chemistry (stability of colloid solutions), biochemistry (cell membranes) and geoenvironmental engineering. Results have been presented at conferences [Refs. 46, 50, 51] and published [Refs. 13, 14, 20, 27].

High pressure phase equilibria and supercritical extraction

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

Vapour–liquid equilibria were determined in four CO_2 + aliphatic alcohol (Me, Et, Pr, iPr) systems around critical conditions. Data are evaluated with use of the SRK equation of state. Model of supercritical extraction was elaborated and description of its hydrodynamics has been further extended. Supercritical extraction of fytosterols, tocoferols, unsaturated fatty acids, beta-caroten from natural raw material was performed experimentally. Results were evaluated with use of the proposed model. Model was applied to data processing of SCF extraction of nettle leaves and schisandra caulomes [Refs. 30, 36–38; see also Department of Diffusion and Separation Processes, Refs. 4, 15, 22–24, 29, 31, 57].

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. 4, 15, 17, 21, 28, 33]

Phase equilibria in reacting systems

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

Experiments: the determinations have been carried out on model systems with esterification reaction, namely acetic acid + alkyl alcohol \leftrightarrow water + alkyl acetate at isothermal conditions (alkyl = methyl, ethyl). New experiments were initiated in studies of transesterification reaction. 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. 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: (a) The Monte Carlo method using simple molecular models combined with the parallel tempering technique was exploited to systematic investigation of solvent driven changes in polymer conformations in a supercritical solvent [Ref. 7]. (b) Gas-liquid equilibria were determined at sub- and supercritical conditions in carbon dioxide + alcohol systems [Refs. 30, 36–38]. (c) Supercritical extraction of fine products from natural raw material was performed experimentally – equilibrium and transport data were determined. Results obtained were correlated with use of the model proposed [see Department of Diffusion and Separation Processes, Refs. 4, 15, 22–24, 29, 31, 57]. (d) Experimental apparatus for determination of the volumetric oxygen mass transfer coefficient in the bubble column using dynamic pressure-step method was fabricated and tested. (e) The vortex structures of impinging jet from a bell-shaped converging nozzle were described, together with the possibilities of their control.

International co-operations

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

University of Agricultural Sciences, Vienna, Austria: Description of liquid-liquid and vapor-liquid equilibria by molecular simulation

University of Ontario, Institute of Technology, Oshawa, Canada: Macroscopic and molecular-based studies in the statistical mechanics of fluids

U. S. Army Research Laboratory, Weapons and Materials Research Directorate, MD, USA

Universitat Rovira i Virgili, Tarragona, Spain: Molecular-based studies of chemically reacting systems in nanoporous materials

Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania: Measurement and prediction of vapour-liquid equilibrium data
ITODYS, University of Paris VII, Paris, France: Vapour-liquid equilibrium bibliographic database; Phase equilibria in selected systems
Oak Ridge Natl. Laboratory, Oak Ridge, USA; Vanderbilt University, Nashville, TN, USA: Simulation of complex fluid systems

Visits abroad

M. Lísal: University of Ontario Institute of Technology, Oshawa, Canada (1 month)
I. Nezbeda: University of Ontario Institute of Technology, Oshawa, Canada (1 month)
L. Vlček: Vanderbilt University, Nashville, TN, USA (2 months)

Visitors

Yu. Kalyuzhnyi, Institute of Condensed Matter Physics, Natl. Acad. Sci. Ukr., Lviv, Ukraine (2 months)
D. Gongalez-Salgado, University of Vigo, Vigo, Spain (3 months)

Teaching

M. Lísal: J. E. Purkyně University, Ústí n. L., courses: "Parallel programming", "Applications of Molecular Simulations", "Numerical mathematics I", "Numerical mathematics II"
I. Nezbeda: J. E. Purkyně University, Ústí n. L., course "Molecular theory of matter"
I. Nezbeda, K. Aim: ICT, postgraduate course "Applied statistical thermodynamics of fluid systems"
I. Nezbeda: J. E. Purkyně University, Ústí n. L., course "Statistical physics I."
I. Nezbeda, M. Předota: CU, course "Introduction to computer simulations in many particle systems"
M. Kotrla, M. Předota: CU, course "Advanced computer simulations in many particle systems"
M. Předota: University of South Bohemia, Č. Budějovice, course "Lectures from physics oriented to particle and nuclear physics"
M. Předota: University of South Bohemia, Č. Budějovice, course "Selected lectures from physics"

Publications

Original papers

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2. Brennan J.K., Lísal M., Gubbins K.E., Rice B.M.: Reaction Ensemble Molecular Dynamics: Direct Simulation of the Dynamic Equilibrium Properties of Chemically Reacting Mixtures. *Phys. Rev. E* 70, 0611031-0611034 (2004).

3. Budinský R., Vacek V., Lísal M.: Vapor-Liquid Equilibria of Alternative Refrigerants and Their Binaries by Molecular Simulations Employing the Reaction Gibbs Ensemble Monte Carlo Method. *Fluid Phase Equilib.* 222-223, 213-220 (2004).
4. Constantinescu D., Wichterle I.: Echilibrul izoterm lichid-vapori in sisteme binare ale alcanilor cu cloroalcani. (Rom) Isothermal Vapour-Liquid Equilibria in Binary Systems Alkane - Chloroalkane. *Rev. Chim. (Bucharest)* 55(2), 108-111 (2004).
5. Lísal M., Aim K., Mecke M., Fischer J.: Revised Equation of State for Two-Center Lennard-Jones Fluids. *Int. J. Thermophys.* 25(1), 159-173 (2004).
6. Lísal M., Brennan J.K., Smith W.R., Siperstein F.R.: Dual Control Cell Reaction Ensemble Molecular Dynamics: A Method for Simulations of Reactions and Adsorption in Porous Materials. *J. Chem. Phys.* 121(10), 4901-4912 (2004).
7. Lísal M., Nezbeda I.: Conformations of Homopolymer Chains and Their Phase Behavior in a Simple Supercritical Solvent. *Fluid Phase Equilib.* 222-223, 247-254 (2004).
8. Lísal M., Nezbeda I., Smith W.R.: Vapor-Liquid Equilibria in Five-Site (TIP5P) Models of Water. *J. Phys. Chem. B* 108(22), 7412-7414 (2004).
9. Lísal M., Smith W.R., Aim K.: Analysis of Henry's Constant for Carbon Dioxide in Water via Monte Carlo Simulation. *Fluid Phase Equilib.* 226, 161-172 (2004).
10. Nezbeda I.: Role of the Range of Intermolecular Interactions in Fluids. *Curr. Opin. Colloid Interface Sci.* 9(1-2), 107-111 (2004).
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12. Nezbeda I., Vlček L.: Thermophysical Properties of Fluids: From Realistic to Simple Models and Their Applications. *Int. J. Thermophys.* 25(4), 1037-1049 (2004).
13. Předota M., Bandura A.V., Cummings P.T., Kubicki J.D., Wesolowski D.J., Chialvo A.A., Machesky M.L.: Electric Double Layer at the Rutile (110) Surface. 1. Structure of Surfaces and Interfacial Water from Molecular Dynamics by Use of ab initio Potentials. *J. Phys. Chem. B* 108(32), 12049-12060 (2004).
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15. Pšutka 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.* 220(2), 161-165 (2004).
16. Roháč V., Růžička K., Růžička V., Zaitsau D.H., Kabo G.J., Diky V., Aim K.: Vapour Pressure of Diethyl Phthalate. *J. Chem. Thermodyn.* 36(11), 929-937 (2004).
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22. Morávková L., Linek J.: Excess Molar Volumes of (Acetophenone + Benzene, or Toluene, or 1,3-Xylene, or 1,3,5-Trimethylbenzene) at Temperatures 298.15 K and 328.15 K. *J. Chem. Thermodyn.*, in press.

23. Morávková L., Linek J.: Excess Molar Volumes of (Propiophenone + Benzene, or Toluene, or Ethylbenzene, or Butylbenzene) at Temperatures 298.15 K and 328.15 K. *J. Chem. Thermodyn.*, in press.
24. Morávková L., Wagner Z., Linek J.: (P, Vm, T) Measurements of (Toluene + Propiophenone) at Temperatures from 298.15 K to 328.15 K and at Pressures up to 40 MPa. *J. Chem. Thermodyn.*, in press.
25. Moučka F., Nezbeda I.: Detection and Characterization of Structural Changes in the Hard-Disk Fluid Near Freezing/Melting Conditions. *Phys. Rev. Lett.*, submitted.
26. Nezbeda I.: Towards a Unified View of Fluids. *Mol. Phys.*, in press.
27. Předota M., Machesky M.L., Wesolowski D.J., Cummings P.T.: Hydrogen Bonding at the Rutile (110) Surface - Aqueous Interface. *CIMTEC Proceedings*, submitted.
28. Psutka Š., Wichterle I.: Isothermal Vapour-Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Propanol, Diisopropyl Ether and 4-Methyl-2-pentanone. *Fluid Phase Equilib.*, submitted.
29. Slovák J., Tanaka H.: Computer Simulation Study of Metastable Ice VII and Amorphous Phases Obtained by Its Melting. *J. Chem. Phys.*, submitted.
30. Teodorescu M., Barhala A., Wichterle I.: The Potential of Soave-Redlich-Kwong Equation of State in Describing Phase Equilibria Data at High Pressures for the CO₂ + 1-Alcohol Systems. *Rev. Roum. Chim.*, submitted.
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Books and monographs

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Chapters in books

34. Smith W.R., Lisal M.: Molecular Simulation of Reaction and Adsorption in Nanochemical Devices: Increase of Reaction Conversion by Separation of a Product from the Reaction Mixture. In: *Computation Science and its Applications - ICCSA 2004*. (Lagana, A., Ed.), pp. 392-401, Springer-Verlag Berlin, Heidelberg 2004.
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Conferences

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38. Babič A., Aim K.: Experimental Study of Vapour-Liquid Equilibria of Binary Systems Carbon Dioxide + Aliphatic Alcohol (Methanol, Ethanol, 1-Propanol, 2-Propanol). 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 2, p. 767, Praha, Czech Republic, 22-26 August 2004.
39. Filáček A., Aim K.: Utilisation of Benchmarking Methodology in the Governance and Management of Research and Development: Experience from the Czech Republic. *RECORD*

- Thematic Network Conference on Benchmarking, Proceedings, p. 91-96, Vienna, Austria, 21-22 January 2004.
40. Linek J., Morávková L.: Temperature Dependence of Excess Molar Volumes in Systems Octane-Aromatic Hydrocarbons. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 2, p. 788, Praha, Czech Republic, 22-26 August 2004.
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 43. Lísal M., Růžička M.: Multiscale Aspects of Fluid Mechanics. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 1110, Praha, Czech Republic, 22-26 August 2004.
 44. Lísal M., Smith W.R., Aim K.: Examination of Henry's Constant for Carbon Dioxide in Water by Monte Carlo Simulations. 10th International Conference on Properties and Phase Equilibria for Product and Process Design, Final Program, p. 154, Snowbird UT, USA, 16-21 May 2004.
 45. Lísal M., Smith W.R., Brennan J.K.: Molecular-Level Simulation of Reacting Systems in Bulk and Confinement. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 2, p. 502, Praha, Czech Republic, 22-26 August 2004.
 46. Machesky M.L., Kubicki J.D., Bandura A.V., Předota M., Wesolowski D.J., Ridley M.K., Bénézeth P.: Hydrogen Bonding and Hydrolysis at the Rutile-Water Interface: Ab initio and Molecular Dynamics Insights and Implications for Surface Complexation Modeling. 227th ACS National Meeting, Posters, p. 70, Anaheim CA, USA, 28 March - 01 April 2004.
 47. Nezbeda I.: Modeling of Polar and Associating Fluid: from Realistic Hamiltonians to Simple Models and their Applications. Computational Modeling and Simulation of Materials, Book of Abstracts, p. 1, Acireale/Catania, Italy, 31 May - 04 June 2004.
 48. Nezbeda I.: On the Effect of the Range of Interactions on the Properties of Fluids: Towards a Unified View of Fluids. NATO Advanced Research Workshop "Ionic Soft Matter", p. 1, Lviv, Ukraine, 14-17 April 2004.
 49. Nezbeda I.: On the Effect of the Range of Interactions on the Properties of Fluids: Towards a Unified View of Fluids. Symposium "Short Range Interactions in Soft Condensed Matter", p. 1, Regensburg, Germany, 26-28 February 2004.
 50. Předota M., Cummings P.T., Wesolowski D.J., Zhang Z., Fenter P., Machesky M.L.: Electric Double Layer at the Rutile (110) Surface: Adsorption of Ions from Molecular Dynamics and X-ray Experiments. 227th ACS National Meeting, Posters, p. 97, Anaheim CA, USA, 28 March - 01 April 2004.
 51. Předota M., Cummings P.T., Wesolowski D.J., Zhang Z., Fenter P., Machesky M.L.: Electric Double Layer at the Rutile (110) Surface. Adsorption of Ions from Molecular Dynamics and X-ray Experiments. 3rd International Conference on Computational Modeling and Simulation of Materials, p. B-7:L12, Acireale, Sicily, Italy, 30 May - 04 June 2004.
 52. Rouha M., Nezbeda I.: Virial Coefficients of Primitive Models of Polar and Associating Fluids. Liquid Matter Workshop 2004, Třešť, Czech Republic, 08-10 October 2004.
 53. Wagner Z., Ždímal V., Smolík J.: Robust Estimation of Particle Size Distribution in Atmospheric Aerosols by Gnostic Theory. International Chemometrics Meeting Chemstat 2004, Conference Proceedings, p. 76-84, Pardubice, Czech Republic, 30 August - 02 September 2004.

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Fields of research

- Catalytic combustion of volatile organic compounds in waste gases
- Transport processes in porous solids
- Sulphide catalysts of unconventional composition
- Unconventional preparation of supported molybdenum catalysts
- Texture of porous solids
- Similarity approach to structure reactivity relationships
- Theoretical analysis of bonding changes and electron correlation in chemical reaction
- Temperature programmed techniques in characterization of catalysts

Applied research

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

Research projects

Study of early ageing of hardened cement paste

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

Physical properties of the hardened cement paste exhibiting a great impact on practice are basically influenced by the nature of its porous structure. Origin of the pores is closely connected with the early stage of hydration process during which the calcium silicate hydrate (CSH) clusters are formed via nucleation and subsequent grows (solidification). This project focuses on the influence of the water to cement ratio both on the induction time of CSH nucleation and on the evolution of porosity in cement gels. The texture properties are correlated together with changes in electrical conductivity and the induction period of calcium silicate hydrates nucleation. [Refs. 37, 56, 62]

Nanostructured materials - texture from physical adsorption

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

Project develops and improves the methods for obtaining textural characteristics (e.g. pore-size distribution-PSD, t-plot) of porous materials from experimental physical adsorption isotherms of various gases. The up-to date evaluation methods are applied together with newly obtained information on adsorbed film thickness. The obtained results are mutually correlated with pore structures established by high-resolution electron microscopy. [Refs. 4, 13, 31, 34, 49, 61-63]

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

(O. Šolcová, supported by GA ASCR, grant No. A4072404)

The project develops and verifies a new method for the determination of diffusion coefficients and other transport characteristics of industrial porous solids with non-standard shapes (which guarantee high outer surface to volume ratio). The chromatographic method in SPSC arrangement is applied. To decrease the number of fitted parameters, the axial dispersion parameter (Peclet number) is obtained independently from responses of SPSC packed with porous pellets with pores blocked by a suitable liquid - Porofil (nonporous packing). The obtained diffusion coefficients and other transport characteristics are compared with characteristics from standard textural analyses. [Refs. 9, 14, 28, 33, 57-59]

Organised materials for highly selective catalytic and separation processes

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

The major focus of the proposed project is on establishing an independent, wide research group involving mostly PhD students and profiting of the cooperation and know how of the applicant's and coapplicants' group in the research areas covered by the topic of the proposal. The team consortium pursues a complex scientific research initially comprising synthesis of catalytic and separation structures, also by methods of nanotechnologies and nanoengineering. The structural and functional characterisation of the processed materials is of primary importance, especially in light of the design of their potential applications. Organised, hierarchically ordered hybrid separation and bifunctional separation/catalytic membranes are targeted. Structural, molecular and process modelling is referred to as an essential part of the project as well. [Refs. 28, 31, 57-60]

Molybdenum sulfide catalysts promoted by platinum metals

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

Effect of acid-base properties of support on activity of the sulfided Rh-Mo catalysts was studied in HDS of thiophene and HDN of pyridine. The supports were amorphous SiO₂-Al₂O₃, Al₂O₃ and MgO. Strong synergetic effects were observed in the HDS irrespectively of the kind of the support. In HDN, a significant effect was observed only on SiO₂-Al₂O₃ catalyst, ascribed to the positive role of acidity [Refs. 10, 64]. The sulfided Mo/Al₂O₃ catalyst was promoted by noble metals such as Rh, Ru, Pd and Pt. The most significant positive effect was observed in HDS after promotion with Rh, Ru and Pd, and in HDN after promotion with Pt [Ref. 11]. This was explained by periodic trends over transition metal sulfides. The effect of Pt and Ru addition to Mo/Al₂O₃ was examined in thiophene HDS and cyclohexene hydrogenation. The Ru promoted catalyst was much better both in HDS and HYD reactions [Ref. 65].

Synergistic effects in hydrodesulfurization and oxidation reactions

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

Temperature programmed techniques were used to characterize physical-chemical properties of the catalysts prepared by impregnation of alumina, TiO₂ or zirconium-modified mesopore silicates with 12-molybdophosphoric acid and with corresponding Fe, Ni and Co salts. Catalytic activity was correlated with the amount of active species reducible in the range 20-500 °C. [Refs. 25-27, 47]

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)

TPR and TPD of CO₂ and NH₃ were used to characterize properties of various calcined hydrotalcite-like Co/Mg-Mn/Al and Ni-(Mg)-MIII (MIII = Al or Mn) compounds. The relations among catalytic activity, reducibility (amount of components reducible in the range 350-450 °C) and basicity (amount of CO₂ desorbed in the same temperature range) were observed. The most active catalyst in the reaction was the Co₄MnAl catalyst. [Refs. 12, 18, 19, 30, 48, 51-53]

New catalytic materials for combustion of VOC and their properties

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

Properties of calcined Ni(Cu)MgMn(Al) hydrotalcite-like compounds were examined and their activity in combustion of model VOC as well. Apart from examination of initial catalytic activities, long-lasting experiments with Ni(Cu)MgMn catalysts were done. We found that sulphates decrease catalytic activity. XPS analysis showed the increase in oxidation state of Mn (from Mn³⁺ to Mn⁴⁺) and Ni as well (Ni²⁺ to Ni³⁺). TPR experiments indicate that CuMgMn system is more resistant to action of higher temperatures than corresponding Ni analogue (NiMgMn). [Refs. 12, 30, 35, 36, 43]

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)

Shaped MgO support of high surface area (307-397 m² g⁻¹), mesoporous texture and good hardness was prepared by hydration/calcination of commercial, low surface area MgO. Nitrogen adsorption isotherms of MgO were compared with isotherms of sol-gel nano-MgO from the literature and with isotherms of typical Al₂O₃ supports. Our MgO exhibited a relatively broad distribution of pores with important amount of pores with diameter above 20 nm. Our MgO exhibited a similar XRD peaks broadening as described in literature for sol-gel nano-MgO. The weight of high surface area MgO increased by about 40% at ambient air, indicating deep hydration of the sample. [Refs. 3, 40-42]

Role of electron pairing in chemical bonds

(R. Ponec, supported by GA ASCR, grant No. IAAA4072403)

The project is a part of longer-term efforts at the systematic exploitation of the pair density as new source of the information about the molecular structure. This density represents the basic theoretical quantity allowing us to describe the behaviour of electron pairs in microscopic system and in past several years the application of this density as well as other related quantities was proven to provide new valuable insights into the role of electron pairing in chemical bonds. Especially useful in this respect was shown to be the so-called domain averaged Fermi holes in terms of which it was possible to elucidate the structure of a wealth of molecules with nontrivial bonding pattern like multicenter bonding, hypervalence,

etc. The main goal of the project is to pursue the systematic exploitation of domain averaged Fermi holes with the main focus on other types of molecules with complex bonding pattern like metal clusters, transition metal complexes, molecules in excited states, etc. [Refs. 6-8, 20-24]

Molecular basis of structure-activity relationships

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

The project is a part of long-term collaboration with the Institute of Computational Chemistry of the University of Girona. The interest in this project is primarily focused on the design of new simple theoretical models and procedures allowing us to build up the microscopic basis both for traditional structure-activity relations as well as for the design of new theoretical QSAR models. [Refs. 2, 5]

Precipitation of ammonium aluminum alum by ammonia

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

Rheology properties of slurries arising during precipitation of ammonium alum by ammonia were studied for various reaction conditions. Higher reaction temperature leads to less viscous slurries.

International co-operations

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

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

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

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

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

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

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

Visitors

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

G. Lendvai, Chemical Institute of Hungarian Academy of Sciences, Budapest, Hungary

R. Palcheva, Institute of Catalysis, Sofia, Bulgaria

Teaching

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

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

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Fields of research

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

Research projects

Multi-scale hydrodynamics of gas-liquid reactors

(M. Růžička, supported by GA CR, grant No.104/04/0827)

The project is focused on the basic research in the hydrodynamic interactions between the phases in gas-liquid reactors and contactors. The basic idea of the project is to decompose the hydrodynamic processes according to their length and time scales, to understand them separately and then to develop a synthetic model for the behaviour of the whole bubbly layer. The research approach combines experimental activity, theoretical modelling, and CFD. The project goal is to find the link between microscale and macroscale. [Refs. 4, 13-17, 22, 33, 38, 63]

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

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

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

biological and polymeric liquids. The related data on diffusivities and viscosities would be an important by-product of the intended research. [Refs. 6, 59, 61-62]

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

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

An experimental study of the near-wall turbulence in the backward-facing step flow is carried out with the aim to cover a wide range of operating parameters (the expansion ratio, the Reynolds number, inlet flow conditions). The electrodiffusion technique is applied to map the wall shear rate and to measure local mass transfer coefficients at the wall. The application of directionally sensitive, multi-segment sensors enables us to determine precisely the position of reattachment and to assess the effect of operation parameters on the size of recirculation zones and the strength of reverse flow close to the wall. These complex measurements provide new information about the behaviour of coherent flow structures in the near-wall region. [Refs. 47, 48, 51, 56]

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. 37, 49, 57]

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. 13-17, 41-46]

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, and 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, microchannel flow, impinging fluid jet, wavy film flow). [Refs. 1-2, 26-27, 61]

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. Three PhD students stayed in our laboratory during the last year. [Refs. 26-27, 34-36, 39, 50, 51]

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 2004: (a) The Monte Carlo method using simple molecular models combined with the parallel tempering technique was exploited to systematic investigation of solvent driven changes in polymer conformations in a supercritical solvent. (b) Gas-liquid equilibria were determined at sub- and supercritical conditions in carbon dioxide + alcohol systems. (c) Supercritical extraction of fine products from natural raw material was performed experimentally - equilibrium and transport data were determined. Results obtained were correlated with use of the model proposed. (d) Experimental apparatus for determination of the volumetric oxygen mass transfer coefficient in the bubble column using dynamic pressure-step method was fabricated and tested [Refs. 11-12]. (e) The vortex structures of impinging jet from a bell-shaped converging nozzle were described, together with the possibilities of their control [Refs. 18-19].

International co-operations

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

Rovira i Virgili University, Tarragona, Spain: Impinging jets

University of Thessaly, Volos, Greece: Liquid film flows

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

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

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

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

Institute of Nuclear Sciences, Belgrade, Serbia and Montenegro: Impinging jets

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

Visits abroad

V. Sobolík: University of La Rochelle, France (12 months)
J. Vejražka: Institute of Fluid Mechanics, Toulouse, France (7 months)

Visitors

M. Blažej, Slovak Technical University, Bratislava, Slovakia (6 months)
F. Huchet, University of Nantes, France (6 months)
V. Bourdette, Rovira i Virgili University, Tarragona, Spain (5 months)
M. Pantzali, Aristotle University, Thessaloniki, Greece (3 months)
S. Vlaev, Institute of Chemical Engineering, BAS, Sofia, Bulgaria
M. Sommerfeld, Martin Luther University, Halle, Germany
A. Tomiyama, S. Hosokawa, Kobe University, Japan

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

1. Deslouis C., Tribollet B., Tihon J.: Near-Wall Turbulence in Drag Reducing Flows Investigated by the Photolithography-Electrochemical Probes. *J. Non-Newtonian Fluid Mech.* 123(2-3), 141-150 (2004).
2. Tihon J.: Hydrodynamics of the Solitary Waves Travelling Down a Liquid. *Fortschr.-Ber. VDI Reihe 3(817)*, 260-269 (2004).
3. Punčochář M., Drahoš J.: Origin of Pressure Fluctuations in Fluidized Beds. *Chem. Eng. Sci.* 60(5), 1193-1197 (2005).
4. Růžička M.: Vertical Stability of Uniform Bubble Chain. *Int. J. Multiphase Flow*, submitted.
5. Vejražka J., Marty P.: Measurement of Temperature Field Using Thermochromic Liquid Crystals. *Int. J. Thermal Sci.*, submitted.
6. Wein O.: Viscometric Flow under Apparent Wall Slip in Parallel-Plate Geometry. *J. Non-Newtonian Fluid Mech.*, submitted.
7. Wein O., Tihon J.: Linear Stability of Inclined Film Flows. *Fluid Dyn. Res.*, submitted.

Patents

8. Hájek M., Drahoš J.: Způsob vysoušení knižního a obdobného papírového materiálu a zařízení k jeho provádění. (Czech) Method of Drying of Book and Similar Paper Material and Equipment for its Processing. Czech. Pat. No. 293280, No. Appl. 2002-4272. Applied: 02.12.30, Granted: 04.01.27.
9. Hájek M., Drahoš J., Volf V., Vosáb J.: Sposob i prístroj dlja termičnoj obrobki materialiv zi skla ta prirodnych materialiv, zokrema vulkaničnogo pochožděnija. (Ukr) Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Volcanic Origin. UA. Pat. No. 2001128712/M/ No. Appl. PCT /CZ00/00042. Applied: 00.06.12, Granted: 04.11.25.
10. Hájek M., Drahoš J., Volf V., Vozáb J.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Volcanic Origin. DE. Pat. No. EP 1228008, No. Appl. 00934849.1. Applied: 00.06.12, Granted: 04.02.11.

Conferences

11. Blažej M., Juraščík M., Markoš J., Drahoš J.: Measurement of Mass Transfer Coefficient in Three Airlift Reactors of Different Scale. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 198, Tatranské Matliare, Slovakia, 24-28 May 2004.
12. Blažej M., Juraščík M., Markoš J., Drahoš J.: Scale Influence on the Volumetric Oxygen Mass Transfer Coefficient in Airlift Reactor with Internal Loop. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 1096, Praha, Czech Republic, 22-26 August 2004.
13. Bunganič R., Růžička M., Drahoš J.: Bubble Formation: High-Speed Images and Acoustic Signals. 3rd International Symposium on Two-Phase Flow Modelling and Experimentation, Final Program, p. 1-3, Pisa, Italy, 22-25 September 2004.
14. Bunganič R., Růžička M., Drahoš J.: Some Aspects of Modelling Gas-Liquid Systems. Topical Problems of Fluid Mechanics 2004, Proceedings, p. 13-14, Prague, Czech Republic, 25 February 2004.
15. Bunganič R., Růžička M., Drahoš J.: High-Speed Images of Bubble Formation. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 922, Praha, Czech Republic, 22-26 August 2004.
16. Bunganič R., Růžička M., Drahoš J.: A Visual and Acoustic Study of Bubble Formation. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 1068, Praha, Czech Republic, 22-26 August 2004.
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20. Czyzak Z., Hoogland H., Allaf K., Sobolík V.: Extraction of Tea Treated by DIC Process. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 2, p. 646, Praha, Czech Republic, 22-26 August 2004.
21. Czyzak Z., Sobolík V., Hoogland H., Allaf K.: Impact of DIC Treatment of Tea Leaves on Their Infusion in Water at Room Temperature. 16es rencontres Agoral Nantes 2004, Book of Abstracts, p. 115-123, Nantes, France, 30 November - 01 December 2004.
22. Drahoš J., Růžička M.: Problems of Time Series Analysis in Characterization of Multiphase Flows. 5th International Conference on Multiphase Flow ICMF-2004, Abstracts, p. K04, Yokohama, Japan, 30 May - 04 June 2004.

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24. Fialová M., Drahoš J.: Effect of Design Parameters, Surfactants and Viscosity on Flow Regime Transition in Bubble Column Reactors. 10th International Summer School of Chemical Engineering, Proceedings, p. 311, Varna, Bulgaria, 24-31 May 2004.
25. Fialová M., Vlaev S.D.: Local Gas Hold-Up Distribution in Perforated Plate Bubble Columns: An Analysis of Contemporary Results. 10th International Summer School of Chemical Engineering, Proceedings, p. 312, Varna, Bulgaria, 24-31 May 2004.
26. Huchet F., Comiti J., Tihon J.: Study of Hydrodynamics and Mass Transfer Inside Crossing Minichannels. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 260, Tatranské Matliare, Slovakia, 24-28 May 2004.
27. Huchet F., Comiti J., Tihon J.: Electrodiffusion Diagnostics of the Flow Inside Crossing Microchannels. Electrochemical Flow Measurements and Microfluidics. COST F2 Concluding Symposium, Abstracts, p. 16, Poitiers, France, 01-03 July 2004.
28. Klíma L., Lefèvre L., Sobolík V., Allaf K.: Conception et realisation d'un reacteur de detente instantanee controlee DIC chauffé par micro-ondes. (Fr) Conception and Realisation of Instantaneous Pressure Drop Reactor DIC Heated by Micro-Waves. 16es rencontres Agoral Nantes 2004, Book of Abstracts, p. 91-98, Nantes, France, 30 November - 01 December 2004.
29. Klíma L., Sobolík V., Allaf K.: Proprietes dielectriques des fruits et des legumes; cas des produits traites par DIC. (Fr) Dielectric Properties of Fruits and Vegetables; Case of Products Treated by DIC. 16es rencontres Agoral Nantes 2004, Book of Abstracts, p. 179-183, Nantes, France, 30 November - 01 December 2004.
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39. Růžička M., Drahoš J., Mena P.C., Teixeira J.A., Thomas N.H.: Small Viscosity Can Stabilize Uniform Bubble Bed. 5th International Conference on Multiphase Flow ICMF-2004, Abstracts, p. 23, Yokohama, Japan, 30 May - 04 June 2004.
40. Růžička M., Drahoš J., Stanovský P., Wichterle K., Thomas N.H.: Bubble Interactions in Vertical Chain. 5th International Conference on Multiphase Flow ICMF-2004, Abstracts, p. 234, Yokohama, Japan, 30 May - 04 June 2004.
41. Stanovský P., Růžička M., Drahoš J., Wichterle K.: Case-Study of Problems Encountered at Small Bubble Formation. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 1095, Praha, Czech Republic, 22-26 August 2004.
42. Stanovský P., Růžička M., Drahoš J., Wichterle K.: Hydrodynamics of Small Bubble Formation: Selected Results. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 94, Tatranské Matliare, Slovakia, 24-28 May 2004.
43. Šimčík M., Blažej M., Růžička M., Drahoš J., Wichterle K.: Bubble Column Simulation with FLUENT. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 1071, Praha, Czech Republic, 22-26 August 2004.
44. Šimčík M., Blažej M., Růžička M., Drahoš J.: A Minireview of CFD Approaches to Multiphase Flow Systems. Topical Problems of Fluid Mechanics, Proceedings, p. 151, Prague, Czech Republic, 25 February 2004.
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47. Tihon J.: Hydrodynamics of the Solitary Waves Travelling Down a Liquid Film. 21st International Congress of Theoretical and Applied Mechanics, Abstract and CD-ROM Proceedings, p. 128, Warsaw, Poland, 15-21 August 2004.
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49. Tihon J.: Flow Visualization in a Liquid Film Flowing Down an Inclined Plane. XIV. Medzinárodná vedecká konferencia Aplikácia experimentálnych a numerických metód v mechanike tekutín, Zborník referátov, p. 77-80, Rajecké Teplice, Slovakia, 28-30 April 2004.
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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)

The verification of degrading potential of selected strains *Pandoraea sp.* was provided. Efficiency of biodegradation of chlorophenols was tested in water solution of individual and mixture of chlorophenols. The research is focused on biodegradation method and catalytic

dehalogenation of chlorophenols and polybrominated diphenylethers on the Pd/Fe catalyst. [Ref. 58]

Bioencapsulation innovation and technologies

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

The method of determination of living and dead immobilized yeast cells based on measurement of intrinsic fluorescence of biogenic fluorophores was developed. In flow-through cuvette fluorescence intensity of intracellular NAD(P)H was monitored during aerobiosis/anaerobiosis transition and correlated with content of dead and living cells. [Refs. 1, 6, 25, 35, 47, 50]

Transformation of liquid polybutadienes to polymeric antidegradants and block copolymers

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

A series of low-molecular-weight polybutadiene-*block*-polydimethylsiloxane-*block*-polybutadiene copolymers has been prepared by a novel coupling of epoxy-telechelic poly(dimethylsiloxanes) with polybutadienyllithium. The coupling was accompanied by formation of homopolymers in only small amounts, which were easily removed by fractional precipitation/centrifugation. The copolymers were characterized by NMR, VPO, SEC and elemental analysis which showed that both butadiene and dimethylsiloxane blocks have narrow molar mass distributions.

Microwave activation of heterogeneous catalytic reactions

(M. Hájek, supported by ICPF)

Research has been focused on the microwave activation of heterogeneous catalytic reactions in liquid phase where reactants are transparent to microwaves and the catalyst is the only compound, which couples with microwaves. It was found that reactions can be efficiently accelerated when the surface of catalyst is superheated and reaction mixture simultaneously cooled. [Refs. 23, 42]

Microwave technology of glass melting

(M. Hájek, supported by GA ASCR, 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. 24, 30, 32-34, 45, 46, 57]

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. New electrodeless lamps have been prepared generating different wavelengths. [Refs. 2, 8, 15, 16]

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. Continuous microwave dryer with capacity of 100 dried books per day has been successfully tested. [Refs. 18, 31, 40, 41, 43, 44]

New cyclization reaction affording dinitrogen heterocycles

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

The cyclization reaction of methyl 3,3,3-trifluoropyruvate leading to trifluoromethylated Peganine, Isaindigotone and Vasicinone analogues has been studied using microwave radiation. It was found that regioselectivity in the lactam ring closure and diastereoselectivity in substituent configuration were affected.

Generation of new compounds for blood substitutes and other biomedical applications

(V. Čírkva, joint project with ICT)

Novel perfluoroalkylated derivatives of D-galactopyranose and xylitol for biomedical uses have been synthesized. Most of the both types of fluoroalkylated carbohydrate derivatives displayed very low level of hemolytic activity and excellent co-emulsifying properties on testing on perfluorodecalin-Pluronic F-68 microemulsions. [Ref. 3]

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)

The synthesis of cyclopentadienes substituted by four polyfluorinated chains starting with new fluorous synthons, bis(perfluoroalkylethyl)acetylenes, were optimized. New Rh(III) and Rh(I) (perfluoroalkyl)tetramethylcyclopentadienyl complexes with phosphine, amine, alkene and diene ligands were synthesized and characterized by NMR. The fluorophilic properties of Ti(IV) complexes were measured. [Refs. 4, 36, 52, 53]

New catalysts based on diphosphinoazine complexes

(J. Čermák, supported by ICPF)

The study 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 completed. The applicability of nickel complexes with diphosphinoazines to catalyze ethylene polymerization was tested in cooperation with Portuguese collaborators. Stoichiometric reactions of selected complexes of diphosphinoazines with Rh(I) and Rh(III) were carried out to find the possibility of their catalytic application. [Refs. 10, 13, 49, 51]

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)

An optical fibre biosensor that uses dichlorotris(1,10-phenantroline)ruthenium(II) hydrate incorporated into adhesive inorganic-organic hybrid polymer coating (ORMOCER®) was constructed. The fluorescence of the complex is quenched by oxygen depletion within the layer, which was linked to glucose by incorporation of enzyme glucose oxidase immobilized on Sepabeads. Optical fibre probes were demonstrated to measure changes in oxygen and glucose concentration in a laboratory bioreactor. [Ref. 14]

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

L. Betancor, Laboratory of Enzyme Technology of the CSCI Madrid, Spain (1 month)
J. Young, University of Manchester, Manchester, Great Britain

Teaching

F. Kaštánek: ICT, course "Bioengineering"
J. Čermák: J. E. Purkyně University, Ústí n. L., courses "Organic Chemistry I" and "Organic Chemistry II"

Publications

Original papers

1. Brányik T., Vicente A.A., Kuncová G., Podrazký O., Dostálek P., Teixeira J.A.: Growth Model and Metabolic Activity of Brewing Yeast Biofilm on the Surface of Spent Grains: A Biocatalyst for Continuous Beer Fermentation. *Biotechnol. Prog.* 6(20), 1733-1740 (2004).
2. Církva V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry II. Photochemistry of 2-tert-Butylphenol. *J. Photochem. Photobiol., A* 168(3), 197-204 (2004).
3. Církva V., Polák R., Paleta O., Kefurt K., Moravcová J., Kodíček M., Forman S.: Novel Perfluoroalkylated Derivatives of D-Galactopyranose and Xylitol for Biomedical Uses Hemocompatibility and Effect on Perfluorocarbon Emulsions. *Carbohydr. Res.* 339(13), 2177-2185 (2004).
4. Čermák Jan, Šťastná L., Sýkora J., Císařová I., Kvíčala J.: Trimethylsilylcyclopentadienes with Polyfluorinated Ponytails and Mono- and Bis(η^5 -cyclopentadienyl)titanium(IV) Complexes Derived from Them. *Organometallics* 23(12), 2850-2854 (2004).
5. Hayer M., Honzátko P., Kašík I., Kostka F., Kuncová G., Matějec V.: Řízení procesu přípravy optických vláken. (Czech) Process Managing of Optic Fibres Preparation. *Telekomunikace* 41(5), 6-11 (2004).
6. Kuncová G., Podrazký O., Ripp S., Trögl J., Sayler G.S., Demnerová K., Vaňková R.: Monitoring of the Viability of Cells Immobilized by Sol-Gel Process. *J. Sol-Gel Sci. Technol.* 31(1-3), 335-342 (2004).
7. Marseaut S., Debourg A., Dostálek P., Votruba J., Kuncová G., Tobin J.M.: A Silica Matrix Biosorbent of Cadmium. *Int. Biodeterior. Biodegrad.* 54(2-3), 209-214 (2004).
8. Müller P., Klán P., Církva V.: The Electrodeless Discharge Lamp: A Prospective Tool for Photochemistry Part 5. Fill Material-Dependent Emission Characteristics. *J. Photochem. Photobiol. A* 171, 51-57 (2004).
9. Schraml J., Hetflejš J., Šabata S., Blechta V., Sýkora J., Roithová J.: Structure of Disilylated Acetoacetoxyhydroxamic Acid. *Collect. Czech. Chem. Commun.* 69(7), 1472-1478 (2004).

10. Storch J., Čermák Jan, Vojtíšek P., Císařová I.: Palladium(II) Amido Complexes with an Unsymmetrical PNP' Pincer-type Coordination and a New (E,E)-Tetradentate Diphosphinoazine Coordination Mode. *Inorg. Chim. Acta* 357(14), 4165-4171 (2004).
11. Tříška J., Kuncová G., Macková M., Nováková H., Paasivirta J., Lahtiperä M., Vrchotová N.: Isolation and Identification of Intermediates from Biodegradation of Low Chlorinated Biphenyls (Delor-103). *Chemosphere* 54(6), 725-733 (2004).
12. Kaštánek F., Demnerová K., Maléterová Y.: Decontamination of Wastewater Contaminated by Polychlorinated Biphenyls. *Water Science and Technology* 50(2), 131-138 (2004).
13. Včelák J., Storch J., Czakóová M., Čermák Jan: Diphosphinoazine Palladium(II) Complexes as Catalysts for the Heck Reaction of Bromides and an Activated Chloride. *J. Mol. Catal.* 222(1-2), 121-126 (2004).
14. Betancor L., López-Gallego F., Hidalgo A., Fuentes M., Podrazký O., Kuncová G., Guisán J.M., Fernández-Lafuente R.: Advantages of the Pre-Immobilization of Enzymes on Pre-Existing Supports for Their Entrapment in Sol-Gels. *Biomacromolecules*, in press.
15. Církva V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry III. Photochemistry of 4-tert-Butylphenol. *J. Photochem. Photobiol., A*, in press.
16. Církva V., Vlková L.: Microwave Photochemistry IV. Preparation of the Electrodeless Discharge Lamps for Photochemical Applications. *J. Photochem. Photobiol., A*, in press.
17. Gavlasová P., Kuncová G., Macková M.: Approaches to Design Whole Cell Biosensors for PCB Analysis Based on Optical Detection. *Biodegradation*, submitted.
18. Hájek M.: Microwave Drying of Paper Documents. *Ceram. Trans.*, submitted.
19. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus D.: Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.*, submitted.
20. Hetflejš J., Šabata S., Podešva J., Netopilík M., Látalová P., Spěváček J.: Synthesis of Triblock Polybutadiene-Poly(dimethylsiloxane) Copolymers by Coupling Reactions. *J. Appl. Polym. Sci.*, submitted.
21. Kaštánek F.: System of Decontamination of Wastes Containing PCBs. *J. Hazard. Mater.*, in press.
22. Kaštánek F., Páca J., Maléterová Y.: Biodegradation of Phenol at the Presence of Polyaromatic Hydrocarbons (PAH) in Soil. *Int. Biodeterior. Biodegrad.*, submitted.
23. Kurfürstová J., Hájek M.: Microwave-Induced Catalytic Transformation of 2-tert-Butylphenol at Low Temperatures. *Res. Chem. Intermed.* 30(6), 673-681 (2004).
24. Murová I., Hájek M., Lovás M.: Využitie mikrovlnnej energie pri chemickej úprave nerastných surovín. (Slov) Application of Microwave Energy in Chemical Modification of Minerals. *Chem. Listy*, in press.
25. Podrazký O., Kuncová G.: Determination of Concentration of Living Immobilized Yeast Cells by Fluorescence Spectroscopy. *Sens. Actuators, B*, in press.
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27. Vlková L., Církva V.: Chlorované fenoly a způsoby jejich degradace. (Czech) Chlorinated Phenols and Methods of Their Degradation. *Chem. Listy*, in press.

Review papers

28. Gavlasová P., Kuncová G., Macková M.: Stanovení PCB - chemické versus biologické metody. (Czech) Determination of PCBs - Chemical Versus Biological Methods. *Biol. listy*, submitted.

Chapters in books

29. Kaštánek F., Kuraš M.: Complex Treatment of Soils Contaminated by Organic Compounds. In: *Coastal Environment V Incorporating Oil Spill Studies*. (Brebbia, C.A. - Saval Perez, J.M., Ed.), pp. 441-448, WIT Press, Southampton 2004.

Patents

30. Hájek M.: Metodo y aparato para el tratamiento termico de materiales de vidrio y materiales naturales, especificamente de origen volcanico. (Span) Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Volcanic Origin. MX. Pat. No. 01/13022. Applied: 01.12.17, Granted: 04.09.28.
31. Hájek M., Drahoš J.: Způsob vysoušení knižního a obdobného papírového materiálu a zařízení k jeho provádění. (Czech) Method of Drying of Book and Similar Paper Material and Equipment for Its Processing. Czech. Pat. No. 293280, No. Appl. 2002-4272. Applied: 02.12.30, Granted: 04.01.27.
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33. Hájek M., Drahoš J., Volf V., Vozáb J.: Method and Apparatus for Heat Treatment of Glass Materials and Natural Materials Specifically of Volcanic Origin. DE. Pat. No. EP 1228008, No. Appl. 00934849.1. Applied: 00.06.12, Granted: 04.02.11.
34. Hájek M., Smrček J., Vilk P.: Method and Apparatus for Homogenisation of Melt. DE. Pat. No. PCT/CZ02/00063. Applied: 02.11.15, Granted: 04.09.15.

Conferences

35. Brányik T., Vicente A.A., Kuncová G., Podrazký O., Teixeira J.A.: Kinetics of Brewing Yeast Accumulation on the Surface of Spent Grains: A Biocatalyst for Brewing Application. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 5, p. 1689, Praha, Czech Republic, 22-26 August 2004.
36. Čermák Jan, Bříza T., Auerová K., Šťastná L., Kvíčala J.: Cyclopentadienes with Fluorous Ponytails - Modifying the Widespread Ligand. 14th International Symposium on Homogeneous Catalysis, Book of Abstracts, p. 292, Munich, Germany, 05-09 July 2004.
37. Francová D., Karhánek D., Kačer P., Storch J., Kuzma M.: Pt(0)Alkene Complexes: Suitable Tool for Study of Surface Phenomena in Heterogeneous Catalysis. XXXVI Symposium on Catalysis, Book of Abstracts, p. 63-64, Prague, Czech Republic, 08-09 November 2004.
38. Gavlasová P., Kuncová G., Macková M.: Bio-Assay Optical Detection of PCBs. 23. Kongres Československé společnosti mikrobiologické, Bulletin, p. 55, Brno, Czech Republic, 06-09 September 2004.
39. Gavlasová P., Kuncová G., Macková M.: The Extended Study of Coloured Intermediates of PCB Degradation by Pseudomonas Species 2. 7th European Conference on Optical Chemical Sensors and Biosensors Europt(r)ode VII, Book of Abstracts, p. 180, Madrid, Spain, 04-07 April 2004.
40. Hájek M.: Microwave Drying of Paper Documents. International Symposium on Microwave Science and Its Application to Related Fields, Proceedings, p. 363-369, Takamatsu, Japan, 27-30 July 2004.
41. Hájek M.: Microwave Drying of Paper Documents. International Conference on Heating by Electromagnetic Sources, Proceedings, Padua, Italy, 22-27 September 2004.
42. Hájek M.: Microwave Chemistry and Specific Effects. ESF PESC Exploratory Workshop, Book of Abstracts, Grazi, Austria, 17-20 September 2004.
43. Hájek M.: Microwave Drying of Paper Documents. Innovative Applikationen der Mikrowellentechnologie in der Oberlainsitz, Tagungsband, p. 101, Zittau, Germany, 05 May 2004.
44. Hájek M.: Microwave Drying of Paper Documents. 4th World Congress on Microwave and Radio Frequency Applications, Proceedings, p. 79, Austin, Texas, USA, 07-12 November 2004.
45. Hájek M.: Microwave Heating of Glass Melts. Glass Trend Workshop on Glass Melting, Eindhoven, Netherlands, 02-03 November 2004.
46. Hájek M., Brustman J.: Basalt Fibers by Microwave Melting. 13th Conference on Electric and Other Highly Efficient Ways of Glass Melting, Book of Abstracts, Plzeň, Czech Republic, 06-08 September 2004.

47. Kuncová G.: Whole Cell Optical Biosensors. The Influence of Immobilization into Silica and Organic/Silica Matrices. 8th World Congress on Biosensors, Abstract Book, p. P2.5.26, Granada, Spain, 24-26 May 2004.
48. Leitmannová E., Storch J., Červený L.: Ru-Complexes as Catalysts for Selective Hydrogenations. XXXVI Symposium on Catalysis, Book of Abstracts, p. 46-47, Prague, Czech Republic, 08-09 November 2004.
49. Matos I., Carvalho M.F.N.N., Čermák Jan, Marques M.M.: Insight into the Catalytic Properties of Ni-Azine Diphosphine for the Polymerization of Ethylene. 14th International Symposium on Homogeneous Catalysis, Book of Abstracts, p. 472, Munich, Germany, 05-09 July 2004.
50. Podrazký O., Kuncová G.: Determination of the Concentration of Living Immobilized Cells by Fluorescence Spectroscopy. 7th European Conference on Optical Chemical Sensors and Biosensors EUROPT(R)ODE VII, Book of Abstracts, p. 63, Madrid, Spain, 04-07 April 2004.
51. Pošta M., Čermák Jan, Vojtíšek P.: Diphosphinoazine Complexes of Rhodium-Synthesis, Structure and Reactivity. XXXVI Symposium on Catalysis, Book of Abstracts, p. 76-77, Prague, Czech Republic, 08-09 November 2004.
52. Šťastná L., Čermák Jan, Sýkora J., Císařová I.: Titanium(IV) Complexes of Fluorinated Trimethylsilylcyclopentadienes. International Networking of Young Scientists, Book of Abstracts, p. 7, Slaný, Czech Republic, 28-30 March 2004.
53. Šťastná L., Čermák Jan, Sýkora J., Císařová I.: Silylcyclopentadienyl Ligands for Fluorous Biphasic Systems. XXXVI Symposium on Catalysis, Book of Abstracts, p. 78, Prague, Czech Republic, 08-09 November 2004.
54. Trögl J., Ripp S., Kuncová G., Sayler G.S., Demnerová K.: Selectivity of the *Pseudomonas fluorescens* HK44 Biosensor. 7th European Conference on Optical Chemical Sensors and Biosensors EUROPT(R)ODE VII, Book of Abstracts, p. 178, Madrid, Spain, 04-07 April 2004.
55. Trögl J., Ripp S., Kuncová G., Sayler G.S., Churavá A., Kubicová L., Demnerová K., Hálová J.: The Use of Immobilized *Pseudomonas fluorescens* HK44 Cells as a Biosensor for Determination of Naphthalene and Salicylate. 23. Kongres Československé společnosti mikrobiologické, Bulletin, p. 119, Brno, Czech Republic, 06-09 September 2004.
56. Tříška J., Paasivirta J., Lahtiperä M., Gavlasová P., Kuncová G.: Biodegradation of Biphenyl as a Model Study for Biodegradation of Its Chlorinated Derivates. 2-(Cyclohex-1-enyl)pyridine as One of the Intermediates and Confirmation of Its Structure by GC-MS Measurement. Sixth Finnish-Russian Seminar: Chemistry and Ecology of Organo-Element Compounds CEOEC'2004, Research Report No. 18, p. 1-2, Jyväskylä, Finland, 14-18 June 2004.
57. Vilks P., Hájek M.: Application of Microwaves in Glass Conditioning. 65th Conference on Glass Problems, Book of Abstracts, p. 6, Columbus, Ohio, USA, 19-20 October 2004.
58. Kaštánek F., Kaštánek P., Maléterová Y.: Decontamination of Waste Water Contaminated by Polychlorinated Biphenyls (PCB). 5th International Congress Chemistry and Chemical Engineering, Programme, p. 241, Habana, Cuba, 18-22 October 2004.
59. Kaštánek F., Vaníček J., Demnerová K.: Experience of the Czech Republic in Biotechnologies. EURO-CASE Workshop: Biotechnology and Society, Vienna, 27-28 October 2004.

Department of Reaction Engineering in Gas Phase

Head: M. Punčochář
Deputy: V. Ždímal

Research groups

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

Aerosol Laboratory

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

Fields of research

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

Research projects

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. 3, 7, 16]

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

(J. Smolik, 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. 5, 12, 34-37]

Particulate matter: Properties related to health effects

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

The project focuses on the development and evaluation of scientific methodologies and databases that would improve the scientific understanding and regulatory basis on the physico-chemical constituents and emission sources of ambient air particulate matter causing the current substantial mortality and morbidity among European populations. [Refs. 20, 33-35]

Indoor aerosol deposition: An experimental study

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

The aim of the project is to study experimentally the deposition of aerosol particles in rectangular cavity at well-defined conditions. The measurements are conducted both with monodispersed and polydispersed aerosols at both low and high aerosol concentrations. Experiments are performed both for still air and turbulent conditions where the influence of ventilation rate, wall roughness, and ambient aerosol infiltrations is investigated. Laboratory tests are compared to the results obtained from measurements in real indoor environment (indoor living space). [Refs. 5, 12, 34-37]

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. 2, 4, 8, 9, 15, 23-26, 28, 30-32]

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

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

Mainly experimental project focusing on development of methods studying nucleation kinetics in supersaturated vapours. It comprises four tasks: (i) Development of a laminar co-flow tube, a device to study binary nucleation using an entirely new method. Flow visualization will be used to find the limits of stability and CFD methods will be applied to compute the flow field. (ii) Improvement of the shock-tube method. (iii) Improvement of the static-diffusion-chamber method. (iv) Testing the experimental setups with selected systems. [Refs. 9, 18, 21, 23, 26-28, 43-45]

Comprehensive size resolved characterization of atmospheric particulate matter in Prague

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

The goal of the project is comprehensive characterization of atmospheric aerosol in Prague. For this purpose concurrent sampling on two sites is performed using cascade impactors, SMPS systems, nano-SMPS and APS together with filter based sampling, yielding particle mass and number size distributions. The relations between size and composition are studied using PIXE, PIGE, INAA, ICP-MS, IC, AAS, and GC-MS analyses. The data together with the available source fingerprints are used in main aerosol sources identification. Further, the relation between aerosol mass and particle number size distributions and composition and atmospheric conditions is also analysed. The project is solved in collaboration with Charles University, Prague and Nuclear Physics Institute AS CR. [Refs. 20, 33, 43]

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. [Refs. 18, 21]

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. [Refs. 19, 42, 44]

International co-operations

- Philipps-University Marburg, Marburg, Germany: Experimental study of homogeneous nucleation in supersaturated vapours
- Finnish Meteorological Institute, Helsinki, Finland: Application of cascade impactors for aerosol studies; Studies on homogeneous nucleation using diffusion chambers
- Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece: Urban aerosols
- 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
- Johns Hopkins University, Baltimore, USA: Light-induced nucleation from supersaturated vapors
- Institute of Physical Chemistry Russian Academy of Sciences, Moscow, Russia: Non-equilibrium phenomena on the solid-gas boundary
- Karpov Institute of Physical Chemistry, Aerosol Department, Moscow, Russia: Nucleation processes studied in diffusion chambers
- Ghent University, Institute for Nuclear Sciences, B-9000 Ghent, Belgium: OC/EC in urban and suburban PM10 aerosol in Prague
- Technion, Haifa, Israel: Deposition of aerosols in lungs

Visitors

- H. Keskinen, Institute of Physics, Tampere University of Technology, Tampere, Finland
- J. M. Mäkelä, Institute of Physics, Tampere University of Technology, Tampere, Finland
- H. Lihavainen, Finnish Meteorological Institute, Helsinki, Finland
- A. P. Hyvärinen, Finnish Meteorological Institute, Helsinki, Finland
- H. Uchtmann, Philipps-University Marburg, Marburg, Germany
- J. L. Katz, Johns Hopkins University, Baltimore, USA
- K. Eleftheriadis, Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece
- S. Vratolis, Institute of Nuclear Technology – Radiation Protection, N.C.S.R. "Demokritos", Athens, Greece
- D. Broday, Technion, Haifa, Israel

Publications

Original papers

1. Hitzenberger R., Berner A., Galambos Z., Maenhaut W., Cafmeyer F., Schwarz J., Müller K., Spindler G., Wieprecht W., Acker K., Hillamo R., Mäkelä T.: Intercomparison of Methods to

- Measure the Mass Concentration of the Atmospheric Aerosol during INTERCOMP2000 – Influence of Instrumentation and Size Cuts. *Atmos. Environ.* 38(38), 6467-6476 (2004).
2. Keskinen H., Moravec P., Smolík J., Levdansky V.V., Mäkelä J.M., Keskinen J.: Preparation of ZrO₂ Fine Particles by CVD Process: Thermal Decomposition of Zirconium tert-Butoxide Vapor. *J. Mater. Sci.* 39(15), 4923-4929 (2004).
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 4. Levdansky V.V., Smolík J., Moravec P.: Polimolekulyarnye plenki na poverkhnosti aerazol'nykh chastits. (Russ) Polymolecular Films on the Surface of Aerosol Particles. *Inzh.-Fiz. Zh.* (Translated into *J. Eng. Phys. Therm.* 77(5), 917-922, 2004) 77(5), 41-45 (2004).
 5. Smolík J., Barták M.: Přehled faktorů ovlivňujících chování aerosolů ve vnitřním prostředí. (Czech) Factors Determining Aerosol Behaviour Indoors. *Ochrana ovzduší* 16(36)(2), 13-18 (2004).
 6. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus D.: Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.*, submitted.
 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.: Critical Size of Aerosol Particles in the Resonance Radiation Field. *Int. Commun. Heat Mass Transfer*, in press.
 9. Levdansky V.V., Smolík J., Moravec P.: Vliyaniye poverkhnostnykh protsessov i vneshnikh polei na yavleniya perenosa i fazovye perekhody v aerazol'nykh sistemakh s nanorazmernymi chastitsami. (Russ) Effect of Surface Processes and External Fields on Transfer Phenomena and Phase Transitions in Aerosol Systems with Nanosize Particles. *Inzh.-Fiz. Zh.* (*J. Eng. Phys. Thermophys.*), 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. *Water, Air, Soil Pollut.*, in press.
 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 Series AB*, in press.
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Chapters in books

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36. Smolík J., Ždímal V., Schwarz J.: Vliv různých domácích aktivit na koncentraci aerosolových částic v bytě. (Czech) Influence of Different Indoor Activities on Aerosol Concentration in an Apartment. Česká aerosolová společnost, Book of Abstracts, p. 27-30, Praha, Czech Republic, 24 November 2004.
37. Smolík J., Ždímal V., Schwarz J., Brus D., Lazaridis M.: Characterisation of Indoor/Outdoor PM in Suburban Area of Prague: Time and Size Resolved PM Concentrations. European Aerosol Conference EAC 2004, Abstracts [Journal of Aerosol Science, S741-S742, 2004], Budapest, Hungary, 06-10 September 2004.
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45. Ždímal V., Růžička M.: Length-Scale Hierarchy in Aerosol Mechanics. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 3, p. 1109, Praha, Czech Republic, 22-26 August 2004.

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

PhD students: M. Šyc, M. Vosecký, P. Hejdová

Fields of research

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

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)

The project investigates the influence of combustion regimes and additives, which were injected into the flue gas, on PCDD/F formation. Further, the possibilities of inhibition of de novo synthetic reactions by changing the matrix composition were investigated. The research was finished this year by the main paper published in Chemosphere dealing with PCDD and PCDF formation in the dependence on reaction time. It was concluded that the ruling mechanism of PCDDs formation by coupling reactions of chlorinated phenols is preferential reaction, which proceeds very quickly as compared with formation of PCDFs or PCBs by other mechanisms. [Refs. 2-4, 7, 12, 14, 16]

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

(M. Punčochář, supported by EUREKA 1P04OE156)

Application of a new revolutionary technology developed by W.L. GORE & Associates, Ltd. to safely destroy dioxins and furans contained in off-gas from a municipal solid waste (MSW) incinerator based on catalytic filtration. In the laboratory scale experiments were found the conditions for the formation of highly chlorinated PCDDs, which have the same atypical fingerprint as compared with non-anthropogenic PCDD. The solution of optimization

of combustion conditions in Liberec MSW incinerator was directed to ammonia concentration reduction after non-catalytic NO_x destruction technology. [Ref. 11]

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

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

The project is motivated by effort to contribute to the development of alternative sources of small and medium power engineering. The project deals, in a complex way, with the problems arising in the gasification of typical biofuels in fluidized bed reactors. Physicochemical characteristics of a series of materials suitable as biofuels have been determined. Special attention is paid to the process leading to the lowering of emissions of persistent organic pollutants, heavy metals, HCl, and NO_x.

International co-operations

Vrije Universiteit Brussels, Brussels, Belgium: Formation of POPs

Vienna University of Technology, Vienna, Austria: Gasification

Visitors

Prof. H. Hofbauer, Vienna University of Technology, Vienna, Austria

Publications

Original papers

1. Jochová M., Punčochář M., Horáček J., Štamberg K., Vopálka D.: Removal of Heavy Metals from Water by Lignite-Based Sorbents. *Fuel*, 83(9), 1197-1203 (2004).
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4. Vlková L., Pekárek V., Pacáková V., Karban J., Bureš M., Štulík K.: Dechlorination Ability of Municipal Waste Incineration Fly Ash for Polychlorinated Phenols. *Chemosphere* 56(10), 935-942 (2004).
5. Punčochář M., Drahoš J.: Origin of Pressure Fluctuations in Fluidized Beds. *Chem. Eng. Sci.* 60(5), 1193-1197 (2005).
6. Hartman M., Trnka O., Svoboda K., Veselý V.: Impediment to Incipient Fluidization in Wet Beds of Porous Nonspherical Particles. *Chem. Eng. Commun.*, in press.
7. Pekárek V., Grabic R., Punčochář M., Ullrich J., Fišerová E., Bureš M.: Effect of Sulphur Dioxide, Hydrogen Peroxide, Sulphuric Acid and Their Mixtures on the De-novo Synthesis of

- PCDD and PCDF in the N₂ + 10% O₂ Atmosphere Under Model Laboratory Conditions. Chemosphere, submitted.
8. 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.
 9. 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, in press.

Patents

10. Veselý V., Trnka O., Hartman M.: Způsob identifikace a řízení režimů fluidující vrstvy zrnitého materiálu. (Czech) Control and Identification of a Regime of the Fluidized Bed. Czech. Pat. No. 293762/PV314-99. Applied: 99.01.29, Granted: 04.05.20.
11. Punčochář M., Gruber V., Veselý V.: Způsob spalování látek obsahujících chlor. (Czech) Method of Incineration of Materials Containing Chlorine. Czech. Pat. No. 294552/2002-590. Applied: 02.02.18, Granted: 04.11.29.

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12. Grabic R., Crhová Š., Pekárek V., Tomšej T.: Combustion and Recent Industrial PCB Sources - Significant or Negligible Contribution to PCB Pollution?. SETAC Europe 14th Annual Meeting, Abstracts, p. M02AM1/05, Prague, Czech Republic, 18-22 April 2004.
13. Gruber V., Punčochář M.: Recovery of Palladium from Multimetallic Solutions Produced by Leaching of Electrochemical Wastes. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 5, p. 1910, Praha, Czech Republic, 22-26 August 2004.
14. Pekárek V.: Semi-Continuous Batch Technology for Persistent Organic Compounds Detoxification. SETAC Europe 14th Annual Meeting, Abstracts, p. WE6PM/03, Prague, Czech Republic, 18-22 April 2004.
15. Veselý V., Punčochář M.: Total PET Recycling. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 222, Tatranské Matliare, Slovakia, 24-28 May 2004.
16. Bureš M., Pekárek V.: Výpočet konformace a termodynamických vlastností bifenyly a chlorovaných bifenyly. (Czech) Calculation of the Conformation and Thermochemical Quantities of Biphenyl and Chlorinated Biphenyls. Mezinárodní slovenský a český kalorimetrický seminář 2004, Sborník příspěvků, p. 37-40, Hotel Repiská, Demänova Dolina, Slovakia, 24-28 May 2004.

Laboratory of Systems with Fluidized Bed and High Temperature Gas Cleaning

Research staff: K. Svoboda, M. Hartman, O. Trnka
PhD student: 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. 1-3, 5, 6]

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. 1, 2, 7, 8]

Evaluation of dynamic states of gas fluidized suspensions via pressure fluctuations

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

Research is oriented to 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, 13]

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, 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 (2 months)

Visitors

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

Teaching

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

Publications

Original papers

1. Pohořelý M., Svoboda K., Hartman M.: Feeding Small Quantities of Particulate Solids. *Powder Technol.* 142(1), 1-6 (2004).
2. Pohořelý M., Svoboda K., Hartman M.: Komůrkový suvný dávkovač sypkých materiálů. (Czech) Slide Feeder of Different Particulate Materials. *Chem. Listy* 98(6), 361-365 (2004).
3. 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 Geodyn. Geomater.* 1(2), 261-274 (2004).
4. 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* 83(7-8), 1095-1103 (2004).
5. Hartman M., Pohořelý M., Trnka O.: Transport Velocities of Different Particulate Materials in Pneumatic Conveying. *Chem. Eng. Sci.*, submitted.
6. Hartman M., Svoboda K., Pohořelý M., Trnka O.: Combustion of Dried Sewage Sludge in a Fluidized-Bed Reactor. *Ind. Eng. Chem. Res.*, submitted.
7. Hartman M., Trnka O., Svoboda K., Veselý V.: Impediment to Incipient Fluidization in Wet Beds of Porous Nonspherical Particles. *Chem. Eng. Commun.*, in press.
8. Hartman M., Trnka O., Šolcová O.: Thermal Decomposition of Aluminium Chloride Hexahydrate. *Ind. Eng. Chem. Res.*, submitted.
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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*, in press.

Review papers

11. Svoboda K.: Tlakové fluidní spalování uhlí, spolu-spalování uhlí se dřevem, emise, výhody a provozní problémy. (Czech) Pressurized Fluidized Bed Combustion of Coal, Co-Combustion of Coal with Wood, Emissions, Advantages and Problems. Zpravodaj ČEA 9(1), 4 (2004).
12. Svoboda K., Fernandez Gutierrez M.-J., Baxter D., Hunter Ch.: N₂O Emissions from Waste and Biomass Incineration Plants. Waste Management, submitted.

Patents

13. Veselý V., Trnka O., Hartman M.: Způsob identifikace a řízení režimů fluidující vrstvy zrnitého materiálu. (Czech) Control and Identification of a Regime of the Fluidized Bed. Czech. Pat. No. 293762/PV314-99. Applied: 99.01.29, Granted: 04.05.20.

Conferences

14. Pohořelý M., Svoboda K., Hartman M., Vošta J.: Emissions of Nitrogen Oxides and Behavior of Heavy Metals in Atmospheric Fluidized Bed Incineration of Dried Sewage Sludge. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 5, p. 1924, Praha, Czech Republic, 22-26 August 2004.
15. Svoboda K., Pohořelý M., Baxter D., Vošta J.: Leaching of Copper from MSWI Bottom Ash, Practical Measures for Improvement and Conditions for Utilization of the Ash as Civil Construction Material. Energy Forum 2004, Proceedings, p. 265-271, Varna, Bulgaria, 11-13 June 2004.
16. Svoboda K., Trnka O., Pohořelý M., Hartman M.: Theoretical Temperatures of Burning Char Particles in Fluidized Bed Combustion. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 205, Tatranské Matliare, Slovakia, 24-28 May 2004.

Laser Chemistry Group

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

Technical staff: D. Bártlová

PhD student: J. Blazevska-Gilev

Fields of research

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

Research projects

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

(J. Pola, supported by GA ASCR, grant No. A 4072107)

IR and UV laser gas-phase co-decomposition of iron pentacarbonyl with acetylene yields Fe clusters incorporated in carbonaceous shell. The laser gas-phase co-decomposition 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. 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, 8, 18]. These reactions can be used for chemical vapour deposition of nanostructured Te and Se films. The IR laser gas-phase co-pyrolysis of iron pentacarbonyl and alkoxyasilane affords chemical vapour deposition of Fe nanoparticles embodied with silicon polymer [Ref. 6]. The solution phase photolysis of ferrocene yields Fe-based nanoparticles accommodated in carbonaceous shell [Ref. 4].

Laser induced deposition of naked and polymer-embedded metal clusters

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

IR laser gas-phase co-pyrolysis of tetramethylgermane and dimethyl telluride affords chemical vapour deposition of nanosized germanium tellurides. The IR laser co-pyrolysis of tetramethyltin and dimethyl telluride affords nanoparticles of tin telluride. Both formations of metal tellurides have been explained by reaction between clusters of the metal and tellurium in hot laser zone. The used method represents a completely novel approach for the synthesis of nanosized inorganic compounds in the gas phase.

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 unique incorporation of TEG into polymerizing CS species [Ref. 2]. UV laser photolysis of CS₂-C₂H₄ mixtures in the gaseous phase represents the first example of copolymerization of carbon disulfide with common monomer and it yields novel polymers in which (CS₂)_n moieties are interlinked with ethylene units [Ref. 9].

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 gaseous butadiyne yields nanostructured polymeric films with high content of sp² hybridized carbon, which are promising candidate materials for EPR oximetry [Ref. 7]. UV laser photolysis of diethylselenium affords thin films of elemental selenium that react with metallic substrates when deposited on them at room temperature to produce metal selenide interlayer. The reaction between bulk metals and selenium phases has been up to now regarded to proceed only at very high temperatures. Our finding thus reveals high reactivity of selenium films towards metals and the possibility of metal selenization at ambient temperatures [Ref. 3].

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

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

MW UV laser photolysis of tetramethyldisilazane and hexamethyldisilazane in the gas phase affords chemical deposition of polycarbosilazane films that undergo hydrolysis in air.

Thermal gravimetry of the deposited materials reveals their capability to serve as precursors for novel silicon carbonitrideoxide films. Different reaction conditions have been tested to obtain polymeric films possessing different reactivity towards hydrolysis. IR laser pyrolytic co-decomposition of alkoxysilane and alkyl borates has been found as a suitable method for synthesis of nanostructured polyborocarbosiloxanes with high content of Si-O-B bonds [Ref. 12].

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

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

IR laser ablation of poly(1,4-phenylene sulphide) results in deposition of polymers with very low content of sulphur. The procedure has been established to have potential for desulfurization of polyaromatic substances [Ref. 15]. IR laser degradation of poly(vinyl acetate) was recognized as a specific process involving several novel decomposition paths (including formation of vinyl acetate) and allowing deposition of crosslinked polar polymeric films [Ref. 17]. IR laser ablation of poly(vinyl chloride) results in the formation of vinyl chloride and deposition of Cl-containing crosslinked polymeric films. Both laser degradations of the poly(vinyls) represent a novel mode of fabrication of polar intractable polymeric films. They are unique processes for degradation of poly(vinyls) into the monomer.

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

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

Nano-magnetic, thermally stable Fe-based composites were obtained by one-step procedure consisting in continuous-wave IR laser-induced and ethylene-sensitized co-pyrolysis of gaseous iron pentacarbonyl and hexamethyldisiloxane in argon. The simultaneously occurring formation of iron from iron pentacarbonyl and that of organosilicon polymer from hexamethyldisiloxane yield iron nanoparticles surrounded by organosilicon polymer shell. The particles were characterized by a number of techniques and revealed to be partially oxidized in air.

Laser-induced decomposition of four-membered silicon heterocycles

(R. Fajgar, supported by ICPF grant No. 6906)

IR laser gas-phase pyrolysis of silacyclobutane and 1,3-disilacyclobutane affords hydrogenated polycarbosilanes with C/Si ratio 1.5-2 and that in the presence of CO affords polycarbosilanes with C/Si ratio close to 1. The latter polycarbosilanes annealed to 750 °C in vacuum yield stoichiometric SiC.

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

(V. Dřínek, supported by ICPF grant No. 6905)

Reactions between selected monomers (e.g. styrene) and solids obtained from silicon monoxide by pulsed laser ablation were studied and accounted for by polymerization of monomers initiated on $\equiv\text{Si}\cdot$ centres.

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

A. Ouchi, National Institute of Materials and Chemical Research, Tsukuba, Japan
N. Herlin, CEA-DSM-DRECAM, Service des Photons, Atomes et Molecules, Saclay, France
M. Santos, 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
A. Kowalewska, Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodź, Poland

Publications

Original papers

1. Dřínek V., Bastl Z., Šubrt J., Pola J.: IR Laser Ablation of Silicon Monoxide in Gaseous Methanol and Hydrocarbons: Deposition of Polyoxocarbosilane. *J. Anal. Appl. Pyrolysis* 71(2), 431-444 (2004).
2. Morita H., Semba K., Bastl Z., Šubrt J., Pola J.: N₂ Laser-Induced Formation of Copolymeric Ultrafine Particles in a Gaseous Tetraethenylgermane-Carbon Disulfide Mixture. *J. Photochem. Photobiol., A* 171, 21-26 (2004).
3. Ouchi A., Bastl Z., Boháček J., Orita H., Miyazaki K., Miyashita S., Bezdička P., Pola J.: Room-Temperature Interaction between Laser-Chemical Vapour-Deposited Selenium and Some Metals. *Chem. Mater.* 16(18), 3439-3445 (2004).
4. Ouchi A., Tsunoda T., Bastl Z., Maryško M., Vorlíček V., Boháček J., Vacek K., Pola J.: Solution Photolysis of Ferrocene into Fe-based Nanoparticles. *J. Photochem. Photobiol., A* 171, 255-260 (2004).
5. 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* 71(2), 635-644 (2004).

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7. Pola J., Ouchi A., Bastl Z., Vacek K., Boháček J., Orita H.: Nanostructured Unsaturated Carbon from Laser-Photo-Polymerization of Diacetylene. *Carbon* 42(12-13), 2521-2526 (2004).
8. Pola J., Pokoná D., Boháček J., Bastl Z., Ouchi A.: Nano-Structured Crystalline Te Films by Laser Gas-Phase Pyrolysis of Dimethyl Tellurium. *J. Anal. Appl. Pyrolysis* 71(2), 739-746 (2004).
9. Tomovska R., Bastl Z., Pola J.: UV Laser Chemical Vapor Deposition of Nano-Chained Copolymer from Carbon Disulfide and Ethene. *Macromol. Chem. Phys.* 205(17), 2239-2245 (2004).
10. 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.* 25(4), 587-591 (2004).
11. Urbanová M., Pola J.: IR Laser Decomposition of 1,3-Disilacyclobutane in Presence of Carbon Disulfide: Chemical Vapour Deposition of Polythiacarbosilane. *J. Organomet. Chem.* 689(16), 2697-2701 (2004).
12. Pola J., Herlin-Boime N., Brus J., Bastl Z., Vacek K., Šubrt J., Vorlíček V.: IR Laser Production of Nano-Structured Polyborocarbosiloxane Powders with Si-O-B Bonds. *Solid State Sci.* 7(1), 123-131 (2005).
13. 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.
14. Dřínek V., Vacek K., Yuzhakov G., Bastl Z.: Interaction between the Silyl and Silylen Centres in the Deposits Prepared by Pulsed Laser Ablation of Silicon Monoxide and Ammonia, Methylamine and Dimethylamine. *Appl. Phys. A*, in press.
15. Durani S.M.A., Khawaja E.E., Masoudi H.M., Bastl Z., Šubrt J., Galíková A., Pola J.: IR Laser Ablative Desulfurization of Poly(1,4-Phenylene Sulfide). *J. Anal. Appl. Pyrolysis*, in press.
16. Fajgar R., Hassler K., Pola J.: Laser Powered Homogeneous Decomposition of 2,2-Diethenylhexamethyltrisilane. *J. Anal. Appl. Pyrolysis*, submitted.
17. Kupčik J., Blazevska-Gilev J., Pola J.: IR Laser-Induced Degradation of Poly(vinyl acetate): Novel Thermal Reactions in the Solid Polymers. *Macromol. Rapid Commun.*, in press.
18. Urbanová M., Pokorná D., Ouchi A., Pola J.: Laser Powered Homogeneous Decomposition of Selenophene and Tellurophene. *J. Anal. Appl. Pyrolysis*, in press.

Patents

19. Ouchi A., Pola J., Bastl Z., Šubrt J., Vorlíček V.: Method to Produce Metal Selenide Thin Film. Pat. No. 2003-10230. Applied: 03.01.17, Granted: 04.08.05.
20. Ouchi A., Pola J., Bastl Z., Vacek K., Šubrt J., Boháček J.: Manufacturing Method for Carbon Materials. Pat. No. JP2004-117330. Applied: 04.04.12.

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21. Dřínek V., Fajgar R., Schneider P., Šnajdaufová H., Šolcová O.: Texture of Silicon Oxycarbide and Silicon Monoxide Powders from Adsorption Measurements. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 166, Tatranské Matliare, Slovakia, 24-28 May 2004.
22. Galíková A., Galík A.: The Study of the Adsorption Kinetics of Acetylene and Methanol on Silica Gel by Gravimetry and Global Fitting. 31st International Conference of Slovak Society of Chemical Engineering, Proceedings, p. 64, Tatranské Matliare, Slovakia, 24-28 May 2004.
23. Pola J.: Laser-Induced Formation of Reactive Species in the Gas Phase: Chemical Vapour Deposition of Novel Polymers. XX IUPAC Symposium on Photochemistry, Book of Abstracts, p. 45, Granada, Spain, 17-22 July 2004.

Department of Analytical Chemistry

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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

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

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

The main aim of this project is to describe how various substituents affect values of $2J(^{29}\text{Si}-^{13}\text{C})$ couplings in the model compounds containing Si-O-C fragment. [Ref. 1]

NMR spectroscopy in solutions

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

Three relatively independent topics are being studied in solution state: ^{29}Si – ^{13}C spin-spin coupling constants, DOSY, and LC-NMR. [Ref. 1]

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.

Enzymatic catalysis in supercritical carbon dioxide

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

LC-NMR identification of the products from enzymatic modifications of blackcurrant seed oil separated by supercritical carbon dioxide continuous-flow extraction. The aim is to develop an integrated production and product recovery process for the extraction from seed and lipase catalysis in supercritical CO₂. [Refs. 9, 15-16]

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. Blechta V., Sýkora J., Schraml J.: Measurement of Long-Range ²⁹Si¹³C Spin-Spin Coupling at Natural Abundance. *Magn. Reson. Chem.* 42(11), 968-972 (2004).
2. Církva V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry II. Photochemistry of 2-tert-Butylphenol. *J. Photochem. Photobiol., A* 168(3), 197-204 (2004).
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4. Karban J., Buděšínský M., Kroutil J.: Synthesis of 1,6-Anhydro-2,3,4-trideoxy-2,3-epimino- and 1,6-Anhydro-2,3,4-trideoxy-3,4-epimino-beta-D-hexopyranoses and Their NMR and Infrared Spectra. *Collect. Czech. Chem. Commun.* 69(10), 1939-1954 (2004).
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8. Schraml J., Sýkora J., Fiedler P., Roithová J., Mindl J., Blechta V., Císařová I., Exner O.: N,O-diacylhydroxylamines—Structures in Crystals and Solutions. *Org. Biomol. Chem.* 2(16), 2311-2314 (2004).
9. Sovová H., Sajfrtová M., Bártlová M., Opletal L.: Near-Critical Extraction of Pigments and Oleoresin from Stinging Nettle Leaves. *J. Supercrit. Fluids* 30(2), 213-224 (2004).
10. Vlková L., Pekárek V., Pacáková V., Karban J., Bureš M., Štulík K.: Dechlorination Ability of Municipal Waste Incineration Fly Ash for Polychlorinated Phenols. *Chemosphere* 56(10), 935-942 (2004).
11. Církva V., Kurfürstová J., Karban J., Hájek M.: Microwave Photochemistry III. Photochemistry of 4-tert-Butylphenol. *J. Photochem. Photobiol., A*, in press.
12. Hetflejš J., Kuncová G., Šabata S., Blechta V., Brus D.: Alternative Synthesis of Poly(hydroxymethylsiloxane) for Lipase Immobilization and Use of the Adsorbates as Esterification Biocatalysts. *J. Sol-Gel Sci. Technol.*, submitted.

13. Jochová M., Punčochář M., Horáček J., Štamberg K., Vopálka D.: Removal of Heavy Metals from Water by Lignite-Based Sorbents. *Fuel*, submitted.
14. Řeřicha R., Blechta V., Soukupová L., Císařová I., Podlaha J., Schraml J.: On Interpretation of a Missing Spectral Band; IR Spectra of Acidic Salts of Benzohydroxamic Acid. *Spectrochim. Acta, Part A*, in press.
15. 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.
16. 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.

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17. Sovová H., Opletal L., Bártlová M., Sajfrtová M.: Solute-Solute and Solute-Matrix Interactions in the Supercritical Fluid Extraction from Plants. 7th Italian Conference on Supercritical Fluids and Their Applications (9th Meeting on Supercritical Fluids), Abstracts, p. 186, Trieste, Italy, 13-16 June 2004.
18. Sovová H., Sajfrtová M., Opletal L., Bártlová M.: Solute-Solute and Solute-Matrix Interactions in the SFE from Plants. 16th International Congress of Chemical and Process Engineering CHISA 2004, Summaries 2, p. 500, Praha, Czech Republic, 22-26 August 2004.
19. Sýkora J., Blechta V., Schraml J.: Measurements of ^{29}Si - ^{13}C Long-Range Coupling Constants. 17th EENC/ 32th AMPERE, PO252, p. PO252, Lille, France, 06-11 September 2004.
20. Sýkora J., Blechta V., Schraml J.: HPLC Coupled to NMR. 19th NMR Valtice, Book of Abstracts, p. 43, Valtice, Czech Republic, 19-21 April 2004.
21. Šťastná L., Čermák Jan, Sýkora J., Císařová I.: Titanium(IV) Complexes of Fluorinated Trimethylsilylcyclopentadienes. International Networking of Young Scientists, Book of Abstracts, p. 7, Slaný, Czech Republic, 28-30 March 2004.
22. Šťastná L., Čermák Jan, Sýkora J., Císařová I.: Silylcyclopentadienyl Ligands for Fluorous Biphasic Systems. XXXVI Symposium on Catalysis, Book of Abstracts, p. 78, Prague, Czech Republic, 08-09 November 2004.

Miscellaneous

International Advisory Board of ICPF

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Memberships in Editorial Boards

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K. Jeřábek: "Reactive and Functional Polymers"
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J. Procházka: "Chemical and Biochemical Engineering"
I. Wichterle: "Chemical Engineering and Technology"
I. Wichterle: "Fluid Phase Equilibria"
V. Ždímal: "Aerosol and Air Quality Research"

Hála Lectures

First (1999)	Arnošt REISER (Polytechnic University, Brooklyn, New York, USA) "Remembering Eduard Hála"
Second (2000)	Gerhart EIGENBERGER (Universität Stuttgart, Stuttgart, Germany) "Membrane Fuel Cell Systems: A Challenge for Chemical Engineers"
Third (2001)	David AVNIR (Hebrew University, Jerusalem, Israel) "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"
- Sixth (2004) Vladimír Hlaváček, (State University of New York, Buffalo, USA)
"Reactivity, Stored Energy, and Dislocations in Solid Reacting Systems"